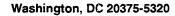
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A Generic Bilevel Formalism for Unifying and Extending Model Reduction Methods

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Multifunctional Materials Branch Materials Science and Technology Division

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13. ABSTRACT (Maximum 200 words)

An abstract, algebraic bilevel version of conventional multigrid methods has been developed that formally unifies and extends the reduced basis, substructuring, smoothing/homogenization, and frequency window methods of model reduction. Within the context of this formalism, a given model reduction method synthesizes a reduced model that plays the role of a "coarse grid" model. Another original-model approximation, conjugate to the model reduction method, plays the role of a "fine grid" model. Conventional multigrid methods can be thought of as an extension of the coarse grid model beyond the original scope of its accuracy through the alternating use of "fine-grid-error-smoothing" and "coarse-grid-correction" steps. Analogously fashioned, abstract versions of these steps extend the particular model reduction method used beyond the original scope of its accuracy. In addition to the development of the mathematical formalism, a generic continuation is proposed and developed as the conjugate approximation for use in the abstract version of the fine-grid-error-smoothing step. For generality, the nature of the parameter-embedding of the continuation is deliberately left unspecified; a particular parameter-embedding is chosen by the analyst to complement the particular model and model reduction method (or class thereof) in a given case. As an example, a particular submethod of this formalism is constructed by specializing the parameter-embedding to a temporal, biscale perturbational parameter-embedding for the case of a generic set of coupled ordinary differential equations with constant coefficients. The initial iteration of this submethod is a general, combined transient/frequency-window methodology for linear finite-element method applications. It is shown to encompass both the force derivative and Lanczos/Ritz vector methods for the limiting case of a zero frequency, singlepoint window for the "fast" time scale. To put this in perspective, the force derivative and Lanczos/Ritz vector methods are two leading approaches for extending/replacing modal reduced basis methods. Current frequency window methods, in turn, are very efficient for extensive time-harmonic reanalysis of the system.

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A GENERIC BILEVEL FORMALISM FOR UNIFYING AND EXTENDING MODEL REDUCTION METHODS

1. INTRODUCTION

In its broadest sense, model reduction methods synthesize, from one model, a new "reduced" model whose response-predictions coincide with that of the original model for a specified subset of the original scope of stimuli. Within this restricted scope of admissible stimuli driving the response, the synthesized model can be used in place of the original model. The benefit usually corresponding to this is a considerable reduction in overall computational effort. This is satisfactory if the modeler/analyst is interested only in the model's response to this subset of admissible stimuli. The problem remains, however, that outside of this restricted scope of admissible stimuli, the synthesized model's predictions typically compare poorly with that of the original model. A remedy to this dramatic dropoff in accuracy is to somehow approximate this "residual" part of the model in a manner that is consistent with the reduced-model synthesized and, at the same time, is complementary to the model reduction method. This results in a hybrid approximation to the original model. "Consistent" here means that the scope over which the reduced model is faithful to the original model is fully preserved when it is combined with the other approximation, conjugate to the model reduction method, to form the hybrid. "Complementary" here means that the conjugate approximation be an adequate one over at least the set of stimuli not admissible to the corresponding model reduction method. A good role model for the combination of complementary approximations into a self-consistent, efficient hybrid is that of multigrid methods [1, 2]. One approximation is effective at eliminating oscillatory error components (on a fine grid) and the other is effective at eliminating smooth error components (on a coarse grid). In this paper, an abstract, algebraic bilevel version of this approach is developed that provides a general means of consistently combining model reduction methods with other approximations. The generic formalism encompasses at least three broad classes of model reduction methods: smoothing/homogenization, reduced basis, and substructuring methods. A particular model reduction method operates at one "level" (the coarse grid analogue) and some conjugate approximation (of the original model response) operates at the other "level" (the fine grid analogue). A generic continuation approach is proposed and developed in this paper as a class of conjugate approximations. This choice is seen to unify and generalize several successful approaches to extending the utility of reduced basis methods.

One important class of model reduction methods applies to the modeling of coupled-multiscale phenomena for which the differences in scale are significant. A prominant example of this would be a structural-component model of a material that possess an intricate spatial heterogeneity of a length scale small with respect to structural dimensions but large with respect to atomic dimensions. Homogenization and smoothing methods of model reduction were developed for these and similar such cases. Both methods refer to the process of mathematically synthesizing a macroscale (usually effective single-phase constitutive) model from a given mesoscale/microscale model such that the predictions of each *coincide* on the macroscale. Methods designed for periodic media are usually referred to as homogenization methods in the literature.

The best known and most widely used is the asymptotic approach [3, 4, 5, 6, 7], which is based on specializing the derivative-expansion version Ref [8, pp. 230–232] of the multiple scales perturbation method to a biscale expansion in the spatial variables. Methods of smoothing (see Refs. [9] and [10, p. 16]), which are designed for statistically homogeneous random media, have several variants, including "self-consistent" methods [10, 11] and methods that bound [10, 12] the constitutive parameter values through the use of variational principles. Fishman and McCoy [13] showed that both homogenization and smoothing methods can be united under a single projection operator framework. Similar projection techniques have been used previously to deduce the influence of one scale upon another in other areas, such as neutron transport Refs. [14, pp. 37, 193-194, and 236-250] and nonequilibrium statistical mechanics [15]. An example of a type of heterogeneity that does not fit either of the usually-assumed periodic or random material models is found in Steinberg and McCoy [16]. They consider the case of fluid-loaded structures for which the heterogeneous regions, each of limited spatial extent on the macroscale, are irregularly distributed. The enabling assumption of the projection technique [13, 16] underlying both homogenization and smoothing methods is that the fluctuation-scale-response is excited solely by its coupling to the macroscale response; any external stimulation of the system is taken to occur at the macroscale only.

Multiscale systems are also represented by models with a finite number of degrees-of-freedom (DOF). If properly chosen, a given subset of the model's DOF can represent a corresponding scale of the model, with fewer DOF usually required the larger the scale. Conventional multigrid methods can be used to model these scales and their coupling for models consisting of sets of algebraic equations. Another important class of finite-degree-of-freedom mathematical models consists of coupled sets of ordinary differential equations, a common source of such models being spatial discretization of a physical system via finite-element methods (FEMs) or finite-difference methods. The number of DOF of such models is often large, making their response-prediction computationally expensive. Two overlapping classes of DOF reduction methods appropriate to such systems are reduced basis methods, which use a Rayleigh-Ritz approximation with respect to a reduced set of generalized coordinates, and "substructuring" methods, for which the DOF of the synthesized reduced-model consists of a chosen subset of the DOF of the original model. The admissible stimuli for the reduced basis method consists of the span of a small number of basis vectors (the "reduced basis"), the number being small compared with the total number of DOF if the method is to be efficient. In turn, the usual enabling assumption for the substructuring methods is that the eliminated DOF, that is, those not retained in the reduced-model (and typically composing the "substructures"), cannot be externally stimulated (loaded). A partial summary of substructuring methods is given by Abdelhamid [17]. The first and still very popular such method is that due to Guyan [18]. Flippen [19] derived a number of such methods from a general time-derivative series solution [20]. The Modal Reduction method [21, 22, 23], popular for the synthesis of Test-Analysis-Models (TAMs) via elimination of (almost) all but the test-sensor-associated DOF, is an adaptation of modal reduced basis methods to substructuring.

For reduced basis methods, the reduced basis sets consist mainly of either Lanczos/Ritz, modal, or solution-path-derivative vectors. As pointed out by Nour-Omid and Clough (Ref. [24, p. 566]), Ritz vector methods [25], as usually implemented, are essentially Lanczos methods. Lanczos methods are applicable to models constrained to loads contained within the span of a small number of fixed vectors. These fixed load-basis vectors are used, in turn, to construct a reduced basis spanning the Krylov subspace associated with the method. The Lanczos method is usually discussed in terms of a second-order formulation, but it also has a first-order formulation [26] for nonproportional damping, as well as block [27], modal-hybrid [28], and other variants. Noting the analogy of their method to those based on Krylov subspaces (in particular, those of Arnoldi and Lanczos), Häggblad and Eriksson [29] recognized that efficient, "generalized Krylov" subspace descriptions can be generated as recursive relations from series solutions of the governing equa-

tions. They take a physical approach and derive advanced methods of this type from series in which "each component is successively computed by balancing the inertia forces from the previous component in the series." This prescription for generating their series is model-specific to mechanics. In particular, they do not explicitly identify an underlying *generic* perturbation or continuation method associated with any of their series. The application of modal reduced basis methods for linear problems is commonplace. Its application has been extended [30] to nonlinear structural dynamics problems as well. Continuation-based reduced basis methods, as summarized mathematically by Rheinboldt (Ref. [31, pp. 80-86]) for example, seem to have a growing history of practical success with respect to some nonlinear problems (see Noor [32], Noor and Whitworth (Ref. [33, p. 915]), Noor (Ref. [34, p. 958]), and Noor and Peters [35], for example). The solution and its path derivatives at a point on the continuation path are used as a Rayleigh-Ritz reduced basis.

Kammer [21] recognized the need for and constructed a hybrid extension to modal reduction for building robust TAMs. The force derivative method is another example of a model reduction hybrid, in this case for extending modal reduced basis approximations. With linear FEM models of mechanical systems as a benchmark, comparisons [36, 37, 38] between several reduced basis methods based on computed responses of the resulting reduced dynamical models, seem to favor the force-derivative [37, 39, 38] and the (closely related) Lanczos [24, 27, 26, 40] methods. This is evidence supporting the utility of hybrid extensions to model reduction methods. The force-derivative method encompasses [39, 38] the older mode-displacement and mode-acceleration methods [41, 42] as zeroth and first-order submethods, respectively. It is essentially a modal basis method that is systematically corrected by terms containing residual mode information. (The chosen modal basis vectors are the target modes whose span contains the reduced model's response.) Its importance is underscored by the fact that it provides both a foundation and extension to the popular Craig-Bampton [43] version of component mode synthesis [44], as shown by Suarez and Singh [45]. The conventional version of the force derivative method is a convolution integral formulation [39, 38], from which higher order corrections are derived via repeated integration by parts of the integral. This integrationby-parts development of the series is apparently serendipitous; a direct systematic development in terms of a generic perturbation methodology is neither mentioned nor used as an alternative. As shown later in this paper, the force derivative and Lanczos methods are closely related. For the case of generic undamped mechanical FEM models, if the force derivative method is constrained to loads within the span of a small number of fixed vectors (a Lanczos requirement), each correction term of the method then reduces to a scalar-multiple of a basis vector for the (Lanczos-associated) Krylov subspace.

Frequency window methods form another class of hybrid methods, their original intention essentially being an extension to modal methods. They are very efficient for extensive time-harmonic re-analysis. In structural acoustics, for example, fine frequency sweeps may be needed to build transient responses (Ref [46, p. 251]) using fast Fourier transforms. Igusa and Achenbach et al. [47, 48, 46] have developed frequency window methods for which substructure attachments are coupled to a main structure by Lagrange multipliers. Its efficiency derives from its use of two complementary approximations, a frequency-response representation of the resonances by simple analytical forms in conjunction with frequency-interpolation over the nonresonance part of the response within a "window." In Ref. [46], for example, the modes of a fluid-loaded shell are used to analyze the response of the same shell with internal substructures. The eigensolution is "subtracted out" of the fluid-shell response, leaving an interpolation over the "smooth," nonresonance part of the fluid-shell response within a window. An analytical expression is used to represent the resonant part of the fluid-shell response in terms of the the fluid-shell eigenvalues and eigenvectors, which are obtained by independent, external means. Flippen [49] developed a frequency window version of substructuring methods for degree-of-freedom reduction. Ingel et al. [50] extended this into a finite-element environment.

The formalism of this paper attempts to encompass these currently accepted, in-use hybrid methods as special limiting cases while mathematically extending their foundation to a more general model reduction setting. In this context, specific computational implementations and applications are beyond the scope of this report. Feedback from such computational experience is ultimately necessary for refining an algoritm and increasing its efficiency. Therefore, the *practical* envelope-of-utility of any particular algorithm arising from this formalism cannot be fully evaluated here.

2. MATHEMATICAL FORMALISM

Let the mathematical model to be considered in this report be generically represented by

$$Lu = f, (2.1)$$

where L is the system operator, u is the system response, and f is the system stimulus (loads, sources, etc.) driving the system. The formal, generic nature of the model description (2.1) allows for the derivation of results of a general nature and utility. It should be noted that (2.1) is not necessarily in a state-space formulation. Although some of the results that follow are not new, they are included for completeness. In addition, the development that follows carries with it the implicit caveat that the ranges and domains of the appropriate operators are such that the various operator compositions indicated are well-defined. As an algebraic notation, juxtapositioning of operators in this report denotes their compositioning as mappings. The additional notation $\mathcal{R}(A) = \{\text{range of } A\}$, $\mathcal{D}(A) = \{\text{domain of } A\}$, and $\mathcal{N}(A) = \{\text{nullspace of } A\}$ for generic operator A will also be used.

2.1 Generalized Inverse Theory for Model Reduction

The typical goal of any particular model reduction method is to provide an accurate approximation to L^{-1} over the "relevant" subsets of possible u's and f's of (2.1), that is, over a restricted domain and range for L. In this report, this approximation to L^{-1} is made *generic* to *all* such model reduction methods and system models (2.1) through the concept of an "outer generalized inverse" of L.

Definition 1 For a given operator L, an outer generalized inverse of L, denoted by L^{I} , satisfies

$$L^I L L^I = L^I. (2.2)$$

Similarly, an "inner generalized inverse" of L, denoted by L^{II} , satisfies

$$LL^{II}L = L. (2.3)$$

The ordinary inverse L^{-1} , when it exists, is both an inner and outer generalized inverse. This report is exclusively concerned with outer generalized inverses. The terminology is borrowed from the theory of matrices (Ref. [51, pp. 428–432]), for which a matrix generalized inverse satisfying both (2.2) and (2.3) always exists for any given matrix L. In a more general operator setting for which L is not necessarily a matrix, one might satisfy one of either (2.2) or (2.3) without satisfying the other. The distinction between which of (2.2) and (2.3) is satisfied is then necessary. The terms "inner" and "outer" are used to make this distinction for lack of a known precedence regarding terminology. As in the matrix case, generalized inverses in this more general setting are *not*, in general, unique. The following theorem also carries over from the matrix case to the general operator setting.

Theorem 1 The operators LL^I and L^IL are each idempotent. If L is bijective, so that L^{-1} exists, then

$$L^{-1} = L^{I} + (I - L^{I}L)L^{-1} (2.4)$$

$$L^{-1} = L^{I} + L^{-1}(I - LL^{I}) (2.5)$$

are identities expressing L^{-1} in terms of L^{I} and a "residual" term containing one of the idempotent operators $(I - L^{I}L)$ or $(I - LL^{I})$.

The proof that LL^I and L^IL are each idempotent follows directly from (2.2). (An idempotent A satisfies $A^2 = AA = A$.) The proof of (2.4) and (2.5) follows from the decompositons of the identity given by

$$I = L^I L + (I - L^I L) (2.6)$$

$$I = LL^{I} + (I - LL^{I}), (2.7)$$

respectively. In (2.6) each element of $\mathcal{D}(L)$ is *uniquely* decomposed into the sum of a component in $\mathcal{R}(L^IL)$ and a component in $\mathcal{R}(I-L^IL)$. Similarly, in (2.7) each element of $\mathcal{R}(L)$ is *uniquely* decomposed into the sum of a component in $\mathcal{R}(LL^I)$ and a component in $\mathcal{R}(I-LL^I)$. If one uses L^I as an approximation to L^{-1} in (2.4) or (2.5) by neglecting the residual term (for now), one is effectively computing a reduced set of responses $\mathcal{R}(L^IL)$ for (2.1) for a reduced set of stimuli $\mathcal{R}(LL^I)$. This can be more easily seen by use of the identities

$$L^{I} = L^{-1}(LL^{I}) (2.8)$$

$$L^{I} = (L^{I}L)L^{-1}. (2.9)$$

The first identity shows that filtering the stimuli in $\mathcal{R}(L)$ by LL^I and then solving (2.1) is equivalent to using L^I directly. Similarly, the second identity shows that filtering the response (obtained from solving (2.1)) by L^IL is also equivalent to using L^I directly.

To make use of outer generalized inverses as model reduction approximations, one must be able to construct them so that either $\mathcal{R}(LL^I)$, $\mathcal{R}(L^IL)$, or both, are adjusted to correspond to the set of relevant stimuli, responses, or both, respectively. The following theorem gives conditions for predetermining $\mathcal{R}(LL^I)$, $\mathcal{R}(L^IL)$, or both for a certain class of outer generalized inverses.

Theorem 2 Given a system operator L for system model (2.1), let the relevant stimuli and response subsets be given by $\mathcal{R}(P_r) \subseteq \mathcal{R}(L)$ and $\mathcal{R}(P_d) \subseteq \mathcal{D}(L)$, respectively, for the linear idempotent operators P_r and P_d . Define the effective version of L as

$$L_{eff} = P_r L P_d. (2.10)$$

If L^{I^*} is defined by

$$L^{I^*} = P_d L_{eff}{}^I P_r, \tag{2.11}$$

then L^{I^*} is an outer generalized inverse of L and

$$\Lambda'(P_rL) \subseteq \mathcal{R}(I - L^{I^*}L). \tag{2.12}$$

For a given f in (2.1), define a model reduction approximation to the response as $u = L^{I^*}f$ for which L_{eff}^I in (2.11) satisfies either

$$P_d L_{eff}{}^I L_{eff} = P_d. (2.13)$$

or

$$L_{\epsilon ff}L_{\epsilon ff}{}^{I}P_{r} = P_{r}. \tag{2.14}$$

or both.

• If L_{eff}^{I} satisfies (2.13) then

$$\mathcal{R}(L^{I^*}L) = \mathcal{R}(P_d)$$

$$= \mathcal{N}(I - L^{I^*}L) \qquad (2.15)$$

$$L^{I^*}LP_d = P_d \qquad (2.16)$$

$$L^{I*}LP_d = P_d (2.16)$$

$$\mathcal{N}(L_{eff}) = \mathcal{N}(P_d). \tag{2.17}$$

• If L_{eff}^{I} satisfies (2.14) then

$$\mathcal{R}(LL^{I^*}) = \mathcal{R}(P_r)$$

$$= \mathcal{N}(I - LL^{I^*})$$

$$P_r LL^{I^*} = P_r$$
(2.18)

$$P_r L L^{I^*} = P_r (2.19)$$

$$\mathcal{N}(P_r L) = \mathcal{R}(I - L^{I^*} L). \tag{2.20}$$

- If $L_{\epsilon f f}^{I}$ satisfies both (2.13) and (2.14), then $L^{I^{*}}$ is unique.
- If P_r and P_d satisfy

$$P_r L(I - P_d) = 0 (2.21)$$

and L_{eff}^{I} satisfies (2.13), then

$$L^{I^*}L = P_d \tag{2.22}$$

and L_{eff}^{I} satisfies (2.14) as well.

• If P_r and P_d satisfy

$$(I - P_r)LP_d = 0 (2.23)$$

and L_{eff}^{I} satisfies (2.14), then

$$LL^{I^*} = P_r. (2.24)$$

If, in addition, $\mathcal{N}(L) = \{0\}$ then $L_{\epsilon ff}{}^I$ satisfies (2.13) as well.

The subscripts "r" and "d" on P_r and P_d denote range and domain (of L), respectively. Appendix A contains the proof of Theorem 2. Theorem 2 reduces the model reduction process to finding a $L_{eff}^{\ \ l}$ satisfying either (2.13) to obtain $\mathcal{R}(L^{I^*}L) = \mathcal{R}(P_d)$ of (2.15), (2.14) to obtain $\mathcal{R}(LL^{I^*}) = \mathcal{R}(P_r)$ of (2.18), or both. The L_{eff} approximation of L given by (2.10) is essentially a generalized Petrov (or Galerkin) method for arbitrary (not necessarily of finite dimension) subspaces.

A primary advantage of satisfying either of the constraints (2.21) or (2.23) is that $L^{I*}f$ may then be an exact solution to (2.1). In the case for which (2.22) is valid, if $u = L^{I^*}f$, then $P_d u = L^{I^*}Lu = L^{I^*}LL^{I^*}f =$ $L^{I^*}f = u$ and $L^{I^*}(Lu - f) = P_du - L^{I^*}f = P_du - u = 0$, so that $(Lu - f) \in \mathcal{N}(L^{I^*})$. In the case for which (2.24) is valid, $f = P_r f = LL^{I^*}f = Lu$ shows that $u = L^{I^*}f$ is an exact solution to (2.1) for all fsatisfying $P_r f = f$.

The constraint (2.23) on P_r and P_d for model reduction is not new. In fact, $P_r L P_d = L P_d$ corresponds exactly with the constraint (6) of (Ref. [52, p. 126]) when making the associations $P_r \to P$ and $P_d \to \Omega P$, where P and ΩP are the notations of (Ref. [52]). The constraint (3) of (Ref. [52, p. 125]) on stimuli fjustifies the association $P_r \to P$. The $P_r L P_d = L P_d$ constraint, in conjunction with (2.14), is seen here to arise naturally as a means of simultaneously obtaining both (2.24) and $\mathcal{R}(L^{I^*}L) = \mathcal{R}(P_d)$ of (2.15) in the case of bijective L. A similar advantage is acrued by adherence to (2.13).

The following corollary of Theorem 2 provides alternatives to (2.4) and (2.5) as decompositions of L^{-1} into L^{I^*} and a residual term.

Corollary 1 If, in Theorem 2, L is bijective then (2.13) implies

$$L^{-1} = L^{I^*} + (I - L^{I^*}L)(I - P_d)L^{-1}$$
(2.25)

and (2.14) implies

$$L^{-1} = L^{I^*} + L^{-1}(I - P_r)(I - LL^{I^*}). {(2.26)}$$

Proof: The relation (2.13) implies (2.16), which implies $(I - L^{I^*}L)P_d = 0$, which in turn implies $(I - L^{I^*}L)(I - P_d) = (I - L^{I^*}L)$, and (2.25) follows from (2.4). The relation (2.14) implies (2.19), which implies $P_r(I - LL^{I^*}) = 0$, which in turn implies $(I - P_r)(I - LL^{I^*}) = (I - LL^{I^*})$, and (2.26) follows from (2.5).

2.2 A Bilevel Formalism

Taking $L^I \to L^{I^*}$ in (2.4) and operating upon f, with $L^{-1}f \approx u_{j+1}$ on the left-hand side and $L^{-1}f \approx u_j$ on the right-hand side, suggests the iteration scheme

$$u_{j+1} = L^{I^*} f + (I - L^{I^*} L) u_j.$$

The iteration error can be found from taking $G \to L^{I^*}$ in the following theorem, which is well-known in matrix iterative analysis.

Theorem 3 Let

$$u_{j+1} = Gf + (I - GL)u_j$$

= $u_j + G(f - Lu_j)$ (2.27)

represent an iteration scheme for u_j for generic G. If the exact error in u_j is given by $e_j = u - u_j$ for $u = L^{-1}f$, then

$$\epsilon_{j+1} = (I - GL)\epsilon_j. \tag{2.28}$$

Proof: Equation (2.27) leads to

$$u_{j+1} = Gf + (I - GL)u_j$$

$$= GL(L^{-1}f) + u_j - GLu_j$$

$$= GLu + u_j - GLu_j$$

$$= GL(u - u_j) + u_j$$

$$= GL\epsilon_j + u_j.$$

so that

$$\epsilon_{j+1} = u - u_{j+1}
= u - u_j - GL\epsilon_j
= \epsilon_j - GL\epsilon_j
= (I - GL)\epsilon_j.$$

As $(I-L^{I^*}L)$ is idempotent, its norm is never less than one, and the iteration scheme does not improve the error with each iteration. As in the multigrid case (see Lemma 2.1 of [1, p. 23]), one needs to combine L^{I^*} with another approximation for L^{-1} . With the *conjugate approximation* for L^{-1} denoted by \widetilde{L}^{-1} , the iterative scheme

$$u_0 = 0 (2.29)$$

$$\tilde{u}_{j+1} = \tilde{L}^{-1} f + (I - \tilde{L}^{-1} L) u_j$$
 (2.30)

$$u_{j+1} = L^{I^*} f + (I - L^{I^*} L) \widetilde{u}_{j+1}$$
 (2.31)

for $j \ge 0$, for which the error satisfies

$$\epsilon_{j+1} = (I - L^{I*}L)(I - \widetilde{L}^{-1}L)\epsilon_j,$$

converges if the norm of $(I - \tilde{L}^{-1}L)$ is sufficiently small. One would expect that if \tilde{L}^{-1} is a "good enough" approximation for L^{-1} , so that $\tilde{L}^{-1}L$ is "close enough" to I, then this norm would be small. If \tilde{L}^{-1} , is a very good approximation for L^{-1} , then one iteration should be a sufficient approximation, so that j=0 in (2.31) leads to

$$L^{-1} \approx L^{I^*} + (I - L^{I^*}L)\tilde{L}^{-1}$$
 (2.32)

upon taking $u_1 \approx L^{-1} f$ on the left-hand side and dropping f (because f is arbitrary). Equation (2.32), or some variant of it based on (2.25) or (2.26), can form the basis of some noniterative model reduction hybrid methods.

The iteration scheme of (2.30) and (2.31) is analogous to a bilevel multigrid method [1, 2], with (2.30) analogous to the fine-grid-smoothing step and (2.31) analogous to the coarse-grid-correction step. The operator $(I-L^{I^*}L)$ is analogous to the coarse-grid-correction matrix. This suggests possible variants of (2.30) and (2.31), such as using *multiple* iterates of (2.30) both before and after the (2.31) iterate, as is usually the case in the conventional bigrid method. Even at this abstract level, the algebraic essence of the bigrid method is preserved in that (2.12) and $\mathcal{N}(I-L^{I^*}L)=\mathcal{R}(P_d)$ of (2.15) are analogous to $\mathcal{N}(I_h^{2h}A^h)\subseteq\mathcal{R}(CG)$ (implied) and $\mathcal{N}(CG)=\mathcal{R}(I_{2h}^h)$, respectively, of Briggs [2, p. 79]. (Both (2.13) and (2.14) are satisfied in the conventional bi-grid method, as will be seen later.)

2.3 Generic Perturbational Conjugate Approximation

A generic continuation approach

$$\widetilde{L}^{-1} = T(\epsilon)^{-1}|_{\epsilon = 0 \to 1} \tag{2.33}$$

for T(1) = L will now be developed as the conjugate approximation of L^{-1} for use in (2.30) or (2.32). As a brief synopsis, in continuation methods one embeds the problem to be solved, denoted generically by

$$T(\overline{\epsilon})u = q(\overline{\epsilon}).$$

into a continuum of problems

$$T(\epsilon)u = q(\epsilon).$$

linked by a parameter, in this case ϵ . The problem to be solved is placed at $\epsilon = \overline{\epsilon}$, where ϵ is usually normalized so that $\overline{\epsilon} = 1$, and a related problem

$$T(0)u = q(0).$$

which is *comparatively* easy to solve, is placed at $\epsilon=0$. There are a number of ways in which the computed continuation from $\epsilon=0$ to $\epsilon=\overline{\epsilon}$ for the generic case can be accomplished [31, 53]. One approach is to carry out a perturbation expansion of the embedded ϵ -problem about $\epsilon=0$, carry a sufficient number of terms in the expansion for accuracy, and evaluate the resulting expansion at $\epsilon=\overline{\epsilon}$. This is an old, widely used version of continuation (Ref. [54, p. 245]), and it is the version that is used in this report (with $\overline{\epsilon}=1$).

If the ϵ expansion of $T(\epsilon)$ is finite for generic operator T, then an explicit, generic perturbational expansion for $T(\epsilon)^{-1}$ is given by the following two theorems.

Theorem 4 Let the operator T have the finite expansion

$$T(\epsilon) = \sum_{j=0}^{J} \epsilon^{j} T_{j}$$
 (2.34)

in the scalar parameter ϵ for a given nonnegative integer J. The linear component operators T_j are each assumed to be independent of ϵ , and T_0^{-1} is assumed to exist. Let the operators Γ^R and Γ^L each have the finite expansions

$$\Gamma^{b}(\epsilon) = \sum_{j=0}^{N} \epsilon^{j} \Gamma^{b}{}_{j}$$
 (2.35)

for a given nonnegative integer $N, b \to R$ or L, where the component operators $\Gamma^R{}_j$ and $\Gamma^L{}_j$ are each assumed to be independent of ϵ . Define the right component operators $\Omega^R{}_j$ by the recursion relation

$$T_0 \Omega^R{}_j = H_{Nj} \Gamma^R{}_j - \left[\sum_{k=1}^J H_{jk} T_k \Omega^R{}_{j-k} \right]$$
 (2.36)

and the left component operators $\Omega^L{}_j$ by the recursion relation

$$\Omega^{L}{}_{j}T_{0} = H_{Nj}\Gamma^{L}{}_{j} - \left[\sum_{k=1}^{J} H_{jk}\Omega^{L}{}_{j-k}T_{k}\right]. \tag{2.37}$$

where the discrete step function H_{jk} is defined by

$$H_{jk} = \begin{cases} I \text{ if } k \le j\\ 0 \text{ if } k > j, \end{cases}$$
 (2.38)

and where I is the identity operator and 0 is the zero operator. The operators

$$\Omega^{R}(\epsilon) = \sum_{i=0}^{M} \epsilon^{j} \Omega^{R}{}_{j}.$$
(2.39)

and

$$\Omega^{L}(\epsilon) = \sum_{j=0}^{M} \epsilon^{j} \Omega^{L}{}_{j}, \tag{2.40}$$

for a given nonnegative integer M, satisfy

$$T\Omega^{R} - \Gamma^{R} = \sum_{j=M+1}^{\mathbf{Max}(N,M+J)} \epsilon^{j} \left[\left(\sum_{k=0}^{J} H_{jk} H_{M,j-k} T_{k} \Omega^{R}_{j-k} \right) - H_{Nj} \Gamma^{R}_{j} \right]$$
(2.41)

and

$$\Omega^{L}T - \Gamma^{L} = \sum_{j=M+1}^{\mathbf{Max}(N,M+J)} \epsilon^{j} \left[\left(\sum_{k=0}^{J} H_{jk} H_{M,j-k} \Omega^{L}_{j-k} T_{k} \right) - H_{Nj} \Gamma^{L}_{j} \right], \tag{2.42}$$

respectively.

Appendix B provides the proof. The above result has utility, for example, when the right-hand sides of (2.41) and (2.42) are $\mathcal{O}(\epsilon^{M+1})$. In this case, (2.41) and (2.42) take the practical forms

$$T\Omega^R - \Gamma^R = \mathcal{O}(\epsilon^{M+1}) \tag{2.43}$$

$$\Omega^L T - \Gamma^L = \mathcal{O}(\epsilon^{M+1}). \tag{2.44}$$

It is assumed that even if the perturbation is not analytical, the results still have value in terms of an asymptotic series. The "of the order of" Landau symbol \mathcal{O} (Ref. [8, p. 8]) is defined by

$$\left\{ \begin{array}{ccc} A(\epsilon) & = & \mathcal{O}(\epsilon^k) \end{array} \right\} & \longleftrightarrow & \left\{ \begin{array}{ccc} \lim_{\epsilon \to 0} \left\| \frac{A(\epsilon)}{\epsilon^k} \right\| & < & \infty \end{array} \right\}$$

for generic A of a normed space with given norm $\| \|$ and a given nonnegative integer k. Sufficient conditions under which Ω^L and Ω^R coincide are provided by the following theorem. (The question as to whether these conditions are also necessary will not be pursued here.)

Theorem 5 Under the hypothesis of Theorem 4 for N=0, assume that (2.36) and (2.37) reduce to

$$\Omega^{R}_{m} = H_{0m}A - \sum_{k=1}^{J} H_{mk}AT_{k}\Omega^{R}_{m-k}$$
(2.45)

and

$$\Omega^{L}_{m} = H_{0m}A - \sum_{k=1}^{J} H_{mk} \Omega^{L}_{m-k} T_{k} A, \qquad (2.46)$$

respectively, for some operator $A = T_0^{-1} \Gamma^R_0 = \Gamma^L_0 T_0^{-1}$. For each $m \ge 0$, the Ω^R_m component of (2.45) and the corresponding Ω^L_m component of (2.46) are *equal*.

The proof is deferred to Appendix C.

2.3.1 Perturbational Operator Inversion

An important special case of the previous section is that for which N=0 and $\Gamma^R=\Gamma^L=\Gamma_0=I$, the identity operator, so that (2.36) and (2.37) reduce to

$$\Omega^{R}_{m} = H_{0m} T_{0}^{-1} - \sum_{k=1}^{J} H_{mk} T_{0}^{-1} T_{k} \Omega^{R}_{m-k}$$
(2.47)

and

$$\Omega^{L}_{m} = H_{0m} T_{0}^{-1} - \sum_{k=1}^{J} H_{mk} \Omega^{L}_{m-k} T_{k} T_{0}^{-1}.$$
(2.48)

respectively, and (2.43) and (2.44) together imply

$$\Omega = T(\epsilon)^{-1} + \mathcal{O}(\epsilon^{M+1}). \tag{2.49}$$

One would expect this to be the case for $T(\epsilon)$ bounded-holomorphic (Ref. [55, pp. 366, 419]), for example. The superscripts R and L have been dropped from the Ω in (2.49) because in this case one has $\Omega^L = \Omega^R$, as supported by the following corollary to Theorem 5.

Corollary 2 Under the hypothesis of Theorem 5 for $\Gamma^R = \Gamma^L = I$, so that $A = T_0^{-1}$, assume that (2.41) and (2.42) imply (2.43) and (2.44), respectively. For each j, the Ω^R_j component of (2.47) and the corresponding Ω^L_j component of (2.48) are equal, so that (2.49) and

$$T(\epsilon)^{-1} = \sum_{j=0}^{M} \epsilon^{j} \Omega_{j} + \mathcal{O}(\epsilon^{M+1})$$
 (2.50)

are justified for Ω_j component operators recursively defined by either (2.47) or (2.48).

Corollary 2 shows that the components given by (2.47) can be thought of as those of the ϵ -expansion of T^{-1} . The *only* inversion used in computing $T(\epsilon)^{-1}$ for all ϵ is that for T_0 .

The results (2.47) can be tested against known results for generic perturbational operator inversions. The J=1 subcase of (2.50), for which (2.47) reduces to

$$\Omega_0 = T_0^{-1} (2.51)$$

$$\Omega_m = [-T_0^{-1}T_1]\Omega_{m-1} \text{ for } m \ge 1,$$
 (2.52)

is equivalent to the well-known Neumann series (Ref. [55, pp. 30, 32]). To see this, take J=1 in (2.34) to get

$$T = T_0 + \epsilon T_1$$

= $T_0 \left[I + \epsilon T_0^{-1} T_1 \right]$
= $T_0 \left[I - \epsilon (-T_0^{-1} T_1) \right]$,

so that

$$T^{-1} = \left[I - \epsilon(-T_0^{-1}T_1)\right]^{-1} T_0^{-1}.$$
 (2.53)

The Neumann series results by the use of the "binomial" operator expansion

$$[I - \epsilon A]^{-1} = \sum_{m=0}^{\infty} \epsilon^m A^m \tag{2.54}$$

for bounded linear operators A (Ref. [56, p. 375]). (The expansion (2.54) is convergent when the magnitude of ϵ is less than the inverse of the norm of A, assuming a Banach space setting.) Using (2.54) with

 $A = -T_0^{-1}T_1$ in (2.53) leads to

$$T^{-1} = \left\{ \sum_{m=0}^{\infty} \epsilon^{m} \left[-T_{0}^{-1} T_{1} \right]^{m} \right\} T_{0}^{-1}$$

$$= \sum_{m=0}^{\infty} \epsilon^{m} \left[-T_{0}^{-1} T_{1} \right]^{m} T_{0}^{-1}$$

$$= \sum_{m=0}^{\infty} \epsilon^{m} \Omega_{m}, \qquad (2.55)$$

where

$$\Omega_m = \left[-T_0^{-1} T_1 \right]^m T_0^{-1}. \tag{2.56}$$

This expression for Ω_m is equivalent to (2.51) and (2.52).

For the J=2 subcase of (2.50), (2.47) leads to

$$\Omega_0 = T_0^{-1} (2.57)$$

$$\Omega_1 = -T_0^{-1} T_1 T_0^{-1} \tag{2.58}$$

$$\Omega_m = -T_0^{-1} [T_1 \Omega_{m-1} + T_2 \Omega_{m-2}] \tag{2.59}$$

for $m \ge 2$. This agrees with the first few terms for T^{-1} given by Kato in (6.16) of (Ref. [55, pp. 420]). Note that (2.57) through (2.59) reduce to (2.51) and (2.52) for $T_2 = 0$, as it should.

2.3.2 Outline of Procedure for Applying Formalism

To complete the development of the generic continuation (2.33) for T(1) = L as the conjugate approximation of L^{-1} , take $\epsilon \to 1$ in (2.50) to get

$$T(\epsilon)^{-1}|_{\epsilon=0\to 1} = \sum_{j=0}^{M} \Omega_j.$$
 (2.60)

As (2.47) or (2.48) are equally valid by Corollary 2, (2.47) will be used for definiteness. With the superscript R dropped from Ω^R in (2.47) because $\Omega^L = \Omega^R$, the Ω_j 's in (2.60) are recursively given by

$$\Omega_m = H_{0m} T_0^{-1} - \sum_{k=1}^J H_{mk} T_0^{-1} T_k \Omega_{m-k}.$$
 (2.61)

The steps to implement the formalism of this paper using this generic perturbation as the conjugate approximation are summarized as:

- Construct the linear idempotent operators P_r and P_d such that the relevant stimuli and response subsets are given by $\mathcal{R}(P_r) \subseteq \mathcal{R}(L)$ and $\mathcal{R}(P_d) \subseteq \mathcal{D}(L)$, respectively, where L is the system operator for the system model (2.1). It is advantageous, but more work, to fix one of either P_r or P_d and determine the other from either (2.21) or (2.23).
- For $L_{\epsilon ff}$ given by (2.10), determine $L_{\epsilon ff}{}^I$ such that it satisfies either (2.13), (2.14), or both. Construct L^{I^*} from this $L_{\epsilon ff}{}^I$ using (2.11).
- Embed L in a ϵ -continuation $T(\epsilon)$ such that

- T_0^{-1} exists
- T_0^{-1} is much more easily computed than L^{-1}
- -T(1) = L, and
- T has the expansion (2.34) for some J.
- The continuation should complement the model reduction approximation L^{I^*} in that it should lead to a reasonably accurate approximation to L^{-1} outside of $\mathcal{R}(P_r)$ and $\mathcal{R}(P_d)$.
- The conjugate approximation \tilde{L}^{-1} is determined by (2.33) and (2.60) for Ω_j 's recursively given by (2.61) for some chosen value of M.
- The solution u to (2.1) is constructed either from $u = L^{-1}f$ with L^{-1} approximated by (2.32), or iteratively using (2.29) through (2.31) (or some variant). There will probably be a tradeoff between M and the number of inner iterations of (2.30); accuracy may require many iterations of (2.30) per evaluation of (2.31) for small M, or only one iteration of (2.30) per evaluation of (2.31) for large enough M.

The next section shows that there are several important classes of model reduction methods for which the second step, in which $L_{\epsilon ff}{}^I$ is determined to satisfy either (2.13), (2.14), or both, is already "worked out." The operator $L_{\epsilon ff}{}^I$ is constructed from $L_{r\epsilon d}{}^{-1}$, where $L_{r\epsilon d}$ is a "reduced" version of L. The construction of $L_{\epsilon ff}{}^I$ from $L_{r\epsilon d}{}^{-1}$ and the specific definition of $L_{r\epsilon d}$ varies from one class of model reduction method to another. For these cases, the bulk of the effort in the second step above reduces to the computational work of obtaining/applying $L_{r\epsilon d}{}^{-1}$.

3. CLASSES OF METHODS ENCOMPASSED

The formalism of this report encompasses the reduced basis, substructuring, and smoothing/homogenization methods of model reduction. To maintain as general a setting as possible for the development of the reduced basis and substructuring methods, L of (2.1) is taken to be a square system matrix with *operator* components, as in Ref. [20]. In keeping with this, the definition of the multiplication of two arbitrary matrices is generalized to

$$(AB)_{ij} = \sum_{k} A_{ik} \circ B_{kj} \tag{3.1}$$

for compatible matrices A and B, where the symbol \circ denotes mapping composition, that is, $A_{ik} \circ B_{kj}$ applied to some function g is interpreted as $A_{ik}(B_{kj}(g))$. The associative and distributive laws of ordinary matrix algebra carry over to this more general setting for the case of linear operator components. For L to preserve compatibility with multiplication by ordinary matrices, and to associate each component of u with one degree-of-freedom, the domain and range of each of the operator components consist of scalar-valued functions. In the special case where B in (3.1) is a matrix of such functions, the \circ in (3.1) is interpreted to mean $A_{ik} \circ B_{kj} = A_{ik}(B_{kj})$. Ordinary matrices are special cases for which each component operator consists of scalar multiplication by a fixed scalar value. Viewed as a single matrix, the L of

$$L = K + D\frac{\partial}{\partial t} + M\frac{\partial^2}{\partial t^2}$$
 (3.2)

is a less trivial example of an operator-component matrix, each component being an ordinary differential equation operator. In mechanics the M, C, and K denote the mass, damping, and stiffness matrices, respectively.

3.1 Reduced Basis Methods

Reduced basis methods consist of an approximation to the original governing equations over subspaces, each of which is spanned by a small number of basis vectors. Let the columns of the matrix Φ_d consist of a set of basis vectors for a chosen subspace of the domain of L. The span of the columns of Φ_d represents the subspace of relevant system responses u for (2.1). Similarly, let the columns of the matrix Φ_r consist of a set of basis vectors for a chosen subspace of the range of L. The span of the columns of Φ_r represents the subspace of relevant system stimuli f for (2.1). The matrices Φ_d and Φ_r are of the same dimensions. The accuracy of any particular reduced basis method is largely dependent on the particular choice of basis in Φ_d and Φ_r , such choice largely distinguishing between specific methods. Let Γ_r and Γ_d be two square matrices whose size is equal to the number of rows of Φ_d and Φ_r , such that $\Phi_r^{\dagger}\Gamma_r\Phi_r$ and $\Phi_d^{\dagger}\Gamma_d\Phi_d$ are both nonsingular. The superscript \dagger denotes the adjoint (transpose with complex conjugation). Take P_r and P_d as

$$P_r = \Gamma_r \Gamma_r^I \tag{3.3}$$

$$P_d = \Gamma_d{}^I \Gamma_d \tag{3.4}$$

for

$$\Gamma_r^I = \Phi_r [\Phi_r^{\dagger} \Gamma_r \Phi_r]^{-1} \Phi_r^{\dagger}$$

$$\Gamma_d^I = \Phi_d [\Phi_d^{\dagger} \Gamma_d \Phi_d]^{-1} \Phi_d^{\dagger}.$$
(3.5)
(3.6)

$$\Gamma_d^I = \Phi_d [\Phi_d^{\dagger} \Gamma_d \Phi_d]^{-1} \Phi_d^{\dagger}. \tag{3.6}$$

Note that $\Gamma_r{}^I$ and $\Gamma_d{}^I$ as defined by (3.5) and (3.6) are outer generalized inverses of Γ_r and Γ_d , respectively. By Theorem 1, P_r and P_d are idempotent as required by Theorem 2. It is also readily shown that

$$\Phi_r^{\dagger} P_r = \Phi_r^{\dagger} \tag{3.7}$$

$$P_d \Phi_d = \Phi_d. \tag{3.8}$$

The $L_{\epsilon ff}$ defined by (2.10) becomes

$$L_{eff} = \Gamma_r \Phi_r [\Phi_r^{\dagger} \Gamma_r \Phi_r]^{-1} L_{red} [\Phi_d^{\dagger} \Gamma_d \Phi_d]^{-1} \Phi_d^{\dagger} \Gamma_d$$
(3.9)

in this case, where the reduced version of L for this class of methods is defined to be

$$L_{red} = \Phi_r^{\dagger} L \Phi_d. \tag{3.10}$$

The size of $L_{r\epsilon d}$ is equal to the number of reduced basis vectors, that is, the number of columns of Φ_r (or Φ_d). The essence of the reduced basis method is to use L_{red}^{-1} instead L^{-1} to solve (2.1). Therefore, the number of such basis vectors must be kept small compared to the original number of DOF for the method to be efficient. The number of Φ_r 's (or Φ_d 's) columns must be significantly less than the number of its rows if worthwhile problem size reduction is to occur.

It is readily verified that L_{eff}^{I} given by

$$L_{eff}^{I} = \Phi_d L_{red}^{-1} \Phi_r^{\dagger} \tag{3.11}$$

is an outer generalized inverse of the L_{eff} of (3.9) that also satisfies

$$L_{eff}^{l}L_{eff} = P_{d} (3.12)$$

$$L_{\epsilon ff}L_{\epsilon ff}{}^I = P_r. {(3.13)}$$

Since P_r and P_d are idempotent, (3.12) and (3.13) imply (2.13) and (2.14), respectively. It is also readily verified that $L^{I^*} = L_{eff}{}^I$ for L^{I^*} given by (2.11), so that

$$L^{I^*} = \Phi_d(\Phi_r^{\dagger} L \Phi_d)^{-1} \Phi_r^{\dagger} \tag{3.14}$$

when (3.10) and (3.11) are used. The classic Rayleigh-Ritz reduced basis approximation consists of (3.14) for the special case of $\Phi_d = \Phi_r = \Phi$, appropriate for self-adjoint L.

3.1.1 Modal Method for Linear Mechanics FEM

As a common and important application of reduced basis methods, consider the linear dynamic mechanics class of finite-element models consisting of second-order ordinary differential equations with real, constant symmetric matrix coefficients. The L of (2.1) becomes (3.2), for which the typical M and K are at least positive, if not positive definite. The modal reduced basis method as typically applied to such systems can be derived as the subcase for which $\Gamma_r = \Gamma_d = M$ and $\Phi_d = \Phi_r = \Phi$, where the columns of Φ are normalized such that

$$\Phi^T M \Phi = I. \tag{3.15}$$

The superscript T denotes the transpose, the matrices being real. For this case, the matrices P_r and P_d reduce to

$$P_r = M\Phi\Phi^T \tag{3.16}$$

$$P_d = \Phi \Phi^T M. \tag{3.17}$$

The modal method is usually accompanied by

- the constraint that $\Phi^T L \Phi$ be diagonal, and
- the constraint (2.23), so that (2.24) is true. This means that $f = P_r f = L(L^{I^*} f)$ for all f in the range of P_r , for which $u = L^{I^*} f$ is an *exact* solution to (2.1).

Substituting (3.16) and (3.17) into (2.23), matrix multiplying the result on the right by Φ , and then using (3.15) on the result gives

$$(I - M\Phi\Phi^T)L\Phi = 0.$$

This leads to

$$K\Phi = M\Phi\Upsilon^2 \tag{3.18}$$

$$C\Phi = M\Phi\beta, \tag{3.19}$$

where

$$\Upsilon^2 = \Phi^T K \Phi \tag{3.20}$$

$$\beta = \Phi^T C \Phi \tag{3.21}$$

for K and C, $(I - M\Phi\Phi^T)M\Phi = 0$ being an *identity* for M by (3.15). The constraint that $\Phi^T L\Phi$ be diagonal reduces to the constraint that Υ^2 and β be diagonal.

If Φ is *determined* so as to satisfy (3.18), then the columns of Φ are eigenvectors satisfying the real eigenproblem (3.18) for which the eigenvalues lie along the diagonal of the diagonal matrix Υ^2 . The eigenvectors are mass normalized by (3.15). (One usually takes Φ such that K and M are positive definite over

the span of the columns of Φ , so that the I in (3.15) and the square of Υ^2 in (3.20) both make sense.) The relation (3.19) is a constraint on C. It can be put into a more conventional form by the following argument. Substituting (3.17) in CP_d leads to $CP_d = M\Phi\beta\Phi^TM$ upon using (3.19). Substituting this into the identity $C = CP_d + C(I - P_d)$ produces the constraint

$$C = (M\Phi)\beta(\Phi^T M) + C(I - P_d)$$
(3.22)

on C. Take (3.21) in (3.19), transpose the result, and then use $C^T = C$, $M^T = M$, and (3.17) to get $\Phi^T C = \Phi^T C (\Phi \Phi^T M) = \Phi^T C P_d$, so that $\Phi^T C (I - P_d) = 0$. Matrix multiplying this on the left by $M\Phi$ gives $P_r C (I - P_d) = 0$ by (3.16), so that the identity $C (I - P_d) = P_r C (I - P_d) + (I - P_r) C (I - P_d)$ gives $C (I - P_d) = (I - P_r) C (I - P_d) = (I - M \Phi \Phi^T) C (I - \Phi \Phi^T M)$. Substituting this into (3.22) and using $M^T = M$ finally leads to the *general* constraint

$$C = (M\Phi)\beta(M\Phi)^T + (I - M\Phi\Phi^T)C(I - M\Phi\Phi^T)^T$$
(3.23)

on the damping matrix. The constraint (3.19) implies that (3.23) and the converse is true as well. If M is nonsingular and one has a complete set of modes, Φ then being square, then one would expect $(I-M\Phi\Phi^T)=0$ in (3.23) and $C=(M\Phi)\beta(M\Phi)^T$. In practice, the $(I-M\Phi\Phi^T)C(I-M\Phi\Phi^T)^T$ component of C is usually neglected, even if one has an incomplete set of modes, so that $C\approx (M\Phi)\beta(M\Phi)^T$. Also, the β matrix is usually specified. A common choice for β in such cases is

$$\beta = 2\zeta \Upsilon, \tag{3.24}$$

where ζ is a diagonal matrix with damping ratio values along its diagonal. Under the condition (3.15) with a complete set of modes, Wilson and Penzien (see (17) through (19) of Ref. [57]) obtain $C = (M\Phi)\beta(M\Phi)^T$ with β given by (3.24). This constraint on C generalizes Rayleigh and proportional damping.

3.1.2 The Conventional Biscale Case of Multigrid

In the biscale case of multigrid methods, the coarse-grid correction is essentially a reduced basis method. Using the notation

$$L \rightarrow L_h$$

$$u \rightarrow u_h$$

$$f \rightarrow f_h$$

of Ref. [1, pp. 18-28], (2.1) represents the fine grid problem. The bigrid coarse-grid correction of Ref. [1, p. 21] is

$$u_h^{j+1} = u_h^j + L^{I*}[f - L_h u_h^j]$$

= $L^{I*}f + (I - L^{I*}L_h)u_h^j$

for L^{I^*} given by

$$L^{I^*} = I_H^h L_H^{-1} I_h^H.$$

This coarse-grid correction is of the form (2.31). The above expression for L^{I^*} implies

$$L^{I^*} = I_H^h (I_h^H L_h I_H^h)^{-1} I_h^H$$

when using

$$L_H = I_h^H L_h I_H^h$$

from (2.21) of Ref. [1, p. 27]. This is in the form of (3.14) upon taking

$$\Phi_d = I_H^h
\Phi_r^{\dagger} = I_h^H.$$

The I_h^H and I_H^h are the restriction and prolongation operators, respectively, required for intergrid information transfer. The matrix-splitting class of error smoothers used in multigrid can be recast as continuation methods. As an example, splitting $L_h = \lambda - U$, where λ is lower triangular and U is upper triangular with zero diagonal, suggests the continuation $T(\epsilon) = \lambda - \epsilon U$ with $T(1) = L_h$. For this case, the zeroth-order $(\epsilon \to 0)$ version of \tilde{L}^{-1} in (2.33) leads to the well-known Gauss-Seidel matrix iterative scheme for (2.30).

3.2 Substructuring Methods

In substructuring methods, one tries to approximate the response of (2.1) for a chosen subset of the DOF of (2.1); this subset being denoted as master DOF. The remaining DOF are correspondingly denoted as the slave DOF. For many substructuring applications, the slave DOF are associated with a collection of substructures that are coupled only through the master DOF, the master DOF being associated with a main coupling structure. Permuting the DOF into master and slave subsets can be represented mathematically by a (real, orthogonal) permutation matrix \mathcal{P} , where

$$\mathcal{P}^T = \mathcal{P}^{-1} \tag{3.25}$$

and the superscript T denotes the transpose. The permutation matrix \mathcal{P} is defined to permute u of (2.1), so that the resulting first \mathcal{M} components of $\mathcal{P}u$, collectively denoted by u_m , are associated with the \mathcal{M} master DOF, and the remaining components, collectively denoted by u_s , are associated with the slave DOF. The convention adopted in this report is that \mathcal{P} , by definition, gathers the master DOF into the upper part of $\mathcal{P}u$, so that

$$\mathcal{P}u = \begin{pmatrix} u_m \\ u_s \end{pmatrix}, \tag{3.26}$$

and similarly for any other column matrix of the same size as u. Using this convention, a choice of substructuring is *completely determined* mathematically by the permutation matrix \mathcal{P} and the number of master DOF \mathcal{M} . This can be extended to square matrices of the size of u as well, and in particular

$$\tilde{L} = \mathcal{P}L\mathcal{P}^{-1}.\tag{3.27}$$

for L leads to the block partitioned form

$$\tilde{L} = \begin{pmatrix} \tilde{L}_{mm} & \tilde{L}_{ms} \\ \tilde{L}_{sm} & \tilde{L}_{ss} \end{pmatrix}. \tag{3.28}$$

That the $L\mathcal{P}^{-1}$ part of (3.27) permutes the columns of L can be seen by $L\mathcal{P}^{-1} = L\mathcal{P}^T = [\mathcal{P}L^T]^T$, where $\mathcal{P}L^T$ permutes the rows of L^T . The \tilde{L}_{mm} of (3.28) is a \mathcal{M} x \mathcal{M} matrix consisting only of those components of L relating master DOF to master DOF. A similar statement is true for \tilde{L}_{ss} with respect to the slave DOF.

From the point of view of this report, substructuring methods are also reduced basis methods but with a different structure from that of Section 3.1. In both cases, the span of the columns of Φ_r determines the subset of $\mathcal{R}(L)$ of 'relevance." In this case, however, the projector P_r satisfies

$$P_r \Phi_r = \Phi_r \tag{3.29}$$

for some choice of Φ_r , as opposed to (3.7). In addition, the admissible Φ_r 's from which one may choose are restricted to a class which is, in some sense, compatible with one's choice of substructuring for the system. This notion is made more precise by the following definition.

Definition 2 For a given number of master DOF \mathcal{M} and a given choice of the permutation matrix \mathcal{P} , let the columns of Φ_r span a subset of $\mathcal{R}(L)$. The reduced basis consisting of the columns of Φ_r is said to be *compatible* with the substructuring \mathcal{M} and \mathcal{P} if

$$\det([\tilde{\Phi}_r]_m^{\dagger}[\tilde{\Phi}_r]_m) \neq 0 \tag{3.30}$$

for the $\mathcal{M} \times \mathcal{K}$ matrix $[\tilde{\Phi}_r]_m$, $1 \leq \mathcal{K} \leq \mathcal{M}$, where

$$\tilde{\Phi}_r = \begin{pmatrix} [\tilde{\Phi}_r]_m \\ [\tilde{\Phi}_r]_s \end{pmatrix} \tag{3.31}$$

for $\tilde{\Phi}_r$ given by

$$\tilde{\Phi}_r = \mathcal{P}\Phi_r. \tag{3.32}$$

The subscripts m and s denote master and slave, respectively.

The following theorem gives this reduced-basis-compatible version of substructuring in the context of the formalism of this report.

Theorem 6 Let the reduced basis consisting of the columns of Φ_r be compatible with the substructuring \mathcal{M} and \mathcal{P} as in Definition 2. Let

$$\Pi_{\gamma} = \begin{pmatrix} I_{mm} & 0 \\ \gamma & 0 \end{pmatrix}$$
(3.33)

represent shorthand notation for a matrix function of its submatrix γ such that square, idempotent Π_{γ} is the same size as L. The I_{mm} of (3.33) is an \mathcal{M} x \mathcal{M} identity matrix. If the matrix α is defined by

$$\alpha = [\tilde{\Phi}_r]_s ([\tilde{\Phi}_r]_m^{\dagger} [\tilde{\Phi}_r]_m)^{-1} [\tilde{\Phi}_r]_m^{\dagger}$$
(3.34)

from (3.31) and (3.32), then the idempotent matrix P_r , defined by

$$P_r = \mathcal{P}^{-1} \Pi_{\alpha} \mathcal{P}. \tag{3.35}$$

satisfies (3.29). If β satisfies

$$[\tilde{L}_{ss} - \alpha \tilde{L}_{ms}]\beta = [\alpha \tilde{L}_{mm} - \tilde{L}_{sm}]. \tag{3.36}$$

then (2.13), (2.14), and (2.23) are satisfied for P_d , L_{red} , and L_{eff}^I given by

$$P_d = \mathcal{P}^{-1} \Pi_{\beta} \mathcal{P}. \tag{3.37}$$

$$L_{red} = \tilde{L}_{mm} + \tilde{L}_{ms}\beta \tag{3.38}$$

$$L_{red} = \hat{L}_{mm} + \hat{L}_{ms}\beta$$

$$L_{eff}^{I} = \mathcal{P}^{-1}\Theta^{I}\mathcal{P}.$$
(3.38)

where

$$\Theta = \begin{pmatrix} L_{red} & 0 \\ 0 & 0 \end{pmatrix}. \tag{3.40}$$

so that

$$\Theta^{I} = \begin{pmatrix} L_{red}^{-1} & 0\\ 0 & 0 \end{pmatrix}. \tag{3.41}$$

In this case, L_{red} is the reduced version of L and L^{I^*} of (2.11) and becomes

$$L^{I^*} = \mathcal{P}^{-1} \Pi_{\beta} \Theta^I \mathcal{P}. \tag{3.42}$$

Appendix D contains the proof. The hypothesis of Theorem 6, if satisfied, implies (2.14) and (2.23), which in turn, by Theorem 2, implies (2.24). As shown previously (just after Theorem 2), (2.24) implies that $L^{I^*}f$ is an exact solution to (2.1) for all f such that $P_rf=f$. The special case of $\alpha=0$ in (3.35) corresponds to conventional substructuring and its variants as currently practiced, with the zero frequency limit corresponding to Guyan condensation. For $\alpha=0$, $P_rf=f$ implies $f=\mathcal{P}^{-1}\Pi_0\mathcal{P}f$, so that

$$f = \mathcal{P}^{-1} \begin{pmatrix} f_m \\ 0 \end{pmatrix}. \tag{3.43}$$

The slave DOF hence cannot be loaded for conventional substructuring if $L^{I^*}f$ is to retain its exact solution status for that case. The idea of using α as in (3.35) and (3.36) has been presented before [52, 20, 49], but its use in connecting reduced basis methods with substructuring methods is emphasized here. There is some similarity in the use of (3.34) for α and the Modal Reduction method (see (10) of Ref. [21, p. 327], for example), which only considers the case in which the reduced basis consists of system modes. The Modal Reduction method, however, builds the reduced system $\Phi^{\dagger}L\Phi$ from the transformation matrix $(I \alpha^T)^T$, and the similarity ends with (3.34).

3.2.1 Reduced-Basis/Substructuring Relationship

If the number of columns of Φ_r is equal to \mathcal{M} , the number of master DOF, then the reduced basis approach of Section 3.1 and the version of substructuring given by Theorem 6 can be directly related to each other.

Theorem 7 Assume the hypothesis of Theorem 6. Take the columns of

$$\Phi_r = \mathcal{P}^{-1} \Pi_{\alpha} \begin{pmatrix} \left[\tilde{\Phi}_r \right]_m \\ 0 \end{pmatrix}, \tag{3.44}$$

as the reduced basis for $\mathcal{R}(L)$, and similarly, take the columns of

$$\Phi_d = \mathcal{P}^{-1} \Pi_\beta \left(\begin{array}{c} [\tilde{\Phi}_d]_m \\ 0 \end{array} \right) \tag{3.45}$$

as the reduced basis for $\mathcal{D}(L)$, where β satisfies (3.36), and $[\tilde{\Phi}_r]_m$ and $[\tilde{\Phi}_d]_m$ are each square and nonsingular. For comparison purposes, denote the substructuring version of L^{I^*} from (3.42) as $L^{I^*}_{sub}$. For Φ_r and Φ_d given by (3.44) and (3.45), respectively, denote the reduced basis version of L^{I^*} from (3.14) as $L^{I^*}_{rb}$. The $L^{I^*}_{rb}$ and $L^{I^*}_{sub}$ are directly related to each other by

$$L_{rb}^{I^{*}} = L_{sub}^{I^{*}} [\Phi_{r} (\Phi_{r}^{\dagger} \Phi_{r})^{-1} \Phi_{r}^{\dagger}].$$
 (3.46)

The proof is deferred to Appendix D. Note that $\Phi_r(\Phi_r^{\dagger}\Phi_r)^{-1}\Phi_r^{\dagger}$ of (3.46) is idempotent. This implies that $L^{I^*}_{rb}$ and $L^{I^*}_{sub}$ coincide over the range of $\Phi_r(\Phi_r^{\dagger}\Phi_r)^{-1}\Phi_r^{\dagger}$. Applying (3.46) to Φ_r and using $[\Phi_r(\Phi_r^{\dagger}\Phi_r)^{-1}\Phi_r^{\dagger}]\Phi_r = \Phi_r$ to the result leads to $L^{I^*}_{rb}\Phi_r = L^{I^*}_{sub}\Phi_r$. This implies that $L^{I^*}_{rb}$ and $L^{I^*}_{sub}$ coincide over the span of the columns of Φ_r .

3.3 Smoothing/Homogenization Methods

Fishman and McCoy (Ref. [13, pp. 47-48]) have unified smoothing and homogenization under one formalism. Proof that the Fishman and McCoy formalism is a subformalism of this report constitutes proof that smoothing and homogenization are encompassed by this report. Smoothing methods presuppose the existence of a "comparison operator" L_0 , a user-chosen approximation to the system operator L of (2.1). The term is taken from applications involving the smoothing of heterogeneous material response in which the L and L_0 typically represent the system operator of a heterogeneous media and an associated "comparison media," respectively. The comparison media is often assumed to be spatially homogeneous with constant constitutive parameters which are "close enough" to the spatially fluctuating ones of L to make the difference between L and L_0 a perturbation. In the abstract case, the comparison operator L_0 is a linear operator that is presumed to satisfy, by definition, the conditions

$$\mathcal{N}(L_0) = \{0\} \tag{3.47}$$

$$L_0P = P_rL_0 (3.48)$$

for P_r of Theorem 2 and P, a linear idempotent operator for which $\mathcal{R}(P) \subseteq \mathcal{D}(L)$. Condition (3.47) guarantees that L_0^{-1} exists. In applications involving the smoothing of the linear response of stochastic heterogeneous materials, for example, the P and P_r are usually both taken to be equal to a common ensemble-averaging projector. A general formalism for smoothing is summarized in the following theorem.

Theorem 8 Let L_0 be a linear operator satisfying the conditions (3.47) and (3.48). Define $\delta L = L - L_0$ for L of (2.1), so that

$$L = L_0 + \delta L. \tag{3.49}$$

If Σ^{-1} exists for

$$\Sigma = L_0 + (I - P_r)\delta L \tag{3.50}$$

and P_d is defined by

$$P_d = [I - \Sigma^{-1}(I - P_r)\delta L]P,$$
 (3.51)

then (2.23) and

$$PP_d = P (3.52)$$

$$P_d^2 = P_d (3.53)$$

$$L_{eff} = \left\{ L_0 + P_r(\delta L) [I - \Sigma^{-1} (I - P_r)(\delta L)] \right\} P$$

= $P_r \left\{ L_0 + [I - (\delta L) \Sigma^{-1} (I - P_r)](\delta L) P \right\},$ (3.54)

for $L_{\epsilon ff}$ given by (2.10).

Corollary 3 Under the hypothesis of Theorem 8, if the constraint

$$P_r(\delta L)P = 0 (3.55)$$

is satisfied, then

$$P_d = [I - \Sigma^{-1} \delta L] P \tag{3.56}$$

$$L_{\epsilon ff} = \left[L_0 - P_r(\delta L) \Sigma^{-1}(\delta L) \right] P$$

$$= P_r \left[L_0 - (\delta L) \Sigma^{-1} (\delta L) P \right] \tag{3.57}$$

for $L_{\epsilon ff}$ given by (2.10).

Proof: Let $G = \Sigma^{-1}(I - P_r)$ so that $\Sigma G = (I - P_r)$, and $0 = P_r(I - P_r) = P_r \Sigma G = P_r[L_0 + (I - P_r)\delta L]G = L_0 PG$ by (3.50) and (3.48). This means that $\mathcal{R}(PG) \subseteq \mathcal{N}(L_0)$, so that PG = 0 by (3.47). This proves

$$P\Sigma^{-1}(I - P_r) = 0. (3.58)$$

Using this and (3.51) in $PP_d = P[I - \Sigma^{-1}(I - P_r)\delta L]P = P$ proves (3.52). Using (3.51) and (3.52) in $P_d^2 = [I - \Sigma^{-1}(I - P_r)\delta L]PP_d = [I - \Sigma^{-1}(I - P_r)\delta L]P = P_d$ proves (3.53). To prove (2.23), take $u \in \mathcal{R}(P_d)$ so that $u = P_d u = [I - \Sigma^{-1}(I - P_r)\delta L]Pu$ by (3.51) and (3.53). (An idempotent operator acts as the identity over its range.) This leads to $(I - P)u = -\Sigma^{-1}(I - P_r)(\delta L)Pu$, so that $\Sigma(I - P)u = -(I - P_r)(\delta L)Pu$. However, $(I - P_r)L(I - P) = (I - P_r)[L_0 + \delta L](I - P) = L_0(I - P) + (I - P_r)\delta L(I - P) = [L_0 + (I - P_r)\delta L](I - P) = \Sigma(I - P)$ by (3.49), $(I - P_r)L_0 = L_0(I - P)$ from (3.48), the idempotent property of P (and of I - P), and (3.50). Substituting this into the previous result gives $(I - P_r)L(I - P)u = -(I - P_r)(\delta L)Pu$. The interim results $P_rL(I - P) = P_r(\delta L)(I - P)$ and $(I - P_r)LP = (I - P_r)(\delta L)P$ follow from $P_rL_0(I - P) = L_0P(I - P) = 0$ and $(I - P_r)L_0P = (I -$

$$L_{eff} = P_r L[I - \Sigma^{-1}(I - P_r)\delta L]P$$

$$= P_r LP - P_r L\Sigma^{-1}(I - P_r)(\delta L)P$$

$$= P_r[L_0 + \delta L]P - P_r L(I - P)\Sigma^{-1}(I - P_r)(\delta L)P$$

$$= L_0 P + P_r(\delta L)P - P_r(\delta L)(I - P)\Sigma^{-1}(I - P_r)(\delta L)P$$

$$= L_0 P + P_r(\delta L)P - P_r(\delta L)\Sigma^{-1}(I - P_r)(\delta L)P$$
(3.59)

when using (3.49), $(I-P)\Sigma^{-1}(I-P_r) = \Sigma^{-1}(I-P_r)$ from (3.58), (3.48), $P_rL(I-P) = P_r(\delta L)(I-P)$, and $(I-P)\Sigma^{-1}(I-P_r) = \Sigma^{-1}(I-P_r)$ again, respectively. The two right-hand sides of (3.54) are just rearrangements of (3.59), where (3.48) was used in the latter.

The $L_{\epsilon ff}$ of Theorem 8 takes either of the forms

$$L_{\epsilon ff} = (L_{red})_d P$$

= $P_r(L_{red})_r$ (3.60)

when defining the reduced system operators

$$(L_{red})_d = L_0 + P_r(\delta L)[I - \Sigma^{-1}(I - P_r)(\delta L)]$$
(3.61)

$$(L_{red})_r = L_0 + [I - (\delta L)\Sigma^{-1}(I - P_r)](\delta L)P,$$
(3.62)

which simplify to

$$(L_{r\epsilon d})_d = L_0 - P_r(\delta L) \Sigma^{-1}(\delta L)$$
(3.63)

$$(L_{r\epsilon d})_r = L_0 - (\delta L) \Sigma^{-1}(\delta L) P \tag{3.64}$$

when (3.55) is satisfied. Define $(L_{\epsilon ff}{}^I)_r$ and $(L_{\epsilon ff}{}^I)_d$ as

$$(L_{eff}^{\ l})_r = (L_{red})_r^{-1} P_r \tag{3.65}$$

$$(L_{eff}^{I})_{d} = P(L_{red})_{d}^{-1}. {(3.66)}$$

so that the choice of $(L_{r\epsilon d})_r$ for the reduced operator leads to

$$L_{eff}(L_{eff}^{I})_{r} = P_{r}, (3.67)$$

which gives (2.14) when operating on (3.67) from the right with P_r . The choice $(L_{red})_d$ leads to

$$(L_{\epsilon ff}{}^{I})_{d}L_{\epsilon ff} = P, (3.68)$$

which gives (2.13) when operating on (3.68) from the left with P_d . Operating on (3.67) on the left by (3.65) shows that $(L_{\epsilon ff}{}^I)_r$ is an outer generalized inverse of $L_{\epsilon ff}$. Similarly, operating on (3.68) on the right by (3.66) shows that $(L_{\epsilon ff}{}^I)_d$ is an outer generalized inverse of $L_{\epsilon ff}$. Taking L^{I^*} from (2.11) leads to

$$L^{I^*} = P_d L_{red}^{-1} P_r (3.69)$$

for generic L_{red} ; that is, either $(L_{red})_r$ or $(L_{red})_d$ can be substituted for L_{red} in (3.69).

If f satisfies the constraint

$$P_r f = f, (3.70)$$

so that $f \in \mathcal{R}(P_r)$, then

$$u = L^{I^*} f (3.71)$$

is possibly an exact solution to (2.1). For the choice of $(L_{red})_r$ as the reduced operator, (2.23) from Theorem 8 and (2.14) together imply (2.24) by Theorem 2. Assuming that $(L_{red})_r^{-1}f$ exists, (2.24) and (3.70) imply that (3.71) is a solution to (2.1). For the choice of $(L_{red})_d$ as the reduced operator, let g be the solution to

$$(L_{red})_d g = P_r f (3.72)$$

subject to the constraint that

$$Pg = g (3.73)$$

so that, if it exists, $g \in \mathcal{R}((L_{red})_d^{-1}P_r) \cap \mathcal{R}(P)$. The problem (3.72) is the "reduced version" of (2.1) for this case. Define u by

$$u = P_d g, (3.74)$$

so that (3.71) follows from (3.69) with $(L_{red})_d$ substituted for L_{red} . Operating on (3.74) on the left by P, using (3.52) on the results to get Pu = Pg, and then substituting g for Pg from (3.73) gives

$$Pu = g. (3.75)$$

The constraint (3.70) and

$$Lu = LP_dg$$

$$= P_rLP_dg$$

$$= L_{\epsilon ff}g$$

$$= (L_{r\epsilon d})_dPg$$

$$= (L_{r\epsilon d})_dg$$

$$= P_rf,$$

which follows from (3.74), (2.23), (2.10), (3.60), (3.73), and (3.72), respectively, show that u is a solution to (2.1).

The formalism of Fishman and McCoy (Ref. [13, pp. 47-48]) is a subformalism of this report corresponding to (3.70), $(L_{red})_d$ as the reduced operator choice, the constraint (3.55),

$$P_r = P ag{3.76}$$

for a special class of P and a specific choice of L_0 . For this case, (3.72) reduces to

$$\{L_0 - P(\delta L)[L_0 + (I - P)\delta L]^{-1}(\delta L)\} P u = f$$
(3.77)

on use of (3.75), (3.70), (3.63), (3.50), and (3.76). Fishman and McCoy use the notation $Pv = \langle v \rangle$ for generic (response or stimulus) $v \in \mathcal{D}(L)$ or $\mathcal{R}(L)$, where $\langle v \rangle$ represents the macroscale component of v. Implicit use of the admissibility test Pf = f, from (3.70) and (3.76), for any given stimulus f is made by Fishman and McCoy Ref. [13, pp. 47-48]; f is a "forcing with variations restricted to the macroscale." This is also true in the formalism of Steinberg and McCoy (Ref. [16, pp. 1135-1136]), as seen by $\langle u_0 \rangle = u_0$ in (19) and (22) of Ref. [16, p. 1135] when making the notational association $f \to u_0$. If P is restricted so as to satisfy the properties

$$P < A > = < A > P \tag{3.78}$$

$$PAP = \langle A \rangle P \tag{3.79}$$

for generic linear operator A, and if L_0 is taken to be

$$L_0 = \langle L \rangle, \tag{3.80}$$

then $PL_0 = L_0P$, corresponding to (3.48) with (3.76), is immediately seen to be true by (3.78). $P(\delta L)P = 0$, corresponding to (3.55) with (3.76), is also true and can be seen by

$$P(\delta L)P = P(L - \langle L \rangle)P$$
= $PLP - P \langle L \rangle P$
= $\langle L \rangle P - \langle L \rangle P^{2}$
= $\langle L \rangle P - \langle L \rangle P$
= 0 .

when using (3.49) and (3.80), (3.78), and (3.79), and $P^2 = P$, respectively. The constraint (3.78) on P corresponds to the constraint (21) of Steinberg and McCoy (Ref. [16, p. 1135]), but it does not seem to be explicitly acknowledged by Fishman and McCoy. The relation (3.77) takes the form

$$\{\langle L \rangle - \langle (\delta L)[\langle L \rangle + (I - P)(\delta L)]^{-1}(\delta L) \rangle\} \langle u \rangle = f$$
(3.81)

when using (3.80), (3.79), and then $Pu \to \langle u \rangle$. Equation (3.81) is exactly the same as the combination of (5) and (6) of Fishman and McCoy (Ref. [13, p. 48]) if the notational adjustment $\delta L \to L'$ is made in (3.81).

4. BISCALE CONJUGATE APPROXIMATION

Consider a class of methods under the umbrella of this formalism for which the ϵ -embedding for the conjugate approximation is based on the premise that there are two relevant time scales, one governing the "fast"

part of the overall response and one governing the "slow" part of the response. Specializing the derivative-expansion version (Ref. [8, pp. 230-232]) of the multiple scales perturbation method to a biscale expansion in time prescribes that

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} \tag{4.1}$$

be substituted for the time derivatives in L to obtain $T(\epsilon)$, where t_0 is the time variable associated with the fast time scale and t_1 is the time variable associated with the slow time scale. (The choice of two scales is based not only on its simplicity and common occurrence, but also that one must be more cautious in the use of the multiple scales approach for three or more scales [58].) This embedding leads to *finite* expansions for $T(\epsilon)$ in ϵ for many common L's, which are *local* in time.

4.1 Frequency Window Variant

A variant of this temporal biscale approach is to use the *Fourier representation* of the t_0 -dependence in the perturbation, so that t_0 -dependence $\to \omega_0$ -dependence. As t_0 is associated with the fast time scale, there should be a "cutoff" value of ω_0 below which the t_1 -dependence dominates. For those cases for which $L(\partial/\partial t)$ satisfies

$$\mathcal{F}_{t_0} L(\frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1}) = L(i\omega_0 + \epsilon \frac{\partial}{\partial t_1}) \mathcal{F}_{t_0}. \tag{4.2}$$

where \mathcal{F}_{t_0} denotes the Fourier transform of the t_0 -dependence into ω_0 -dependence, the continuation is taken to be

$$T(\epsilon, \omega_0) = L(i\omega_0 + \epsilon \frac{\partial}{\partial t_1}). \tag{4.3}$$

Substituting $T(\epsilon, \omega_0)$ of (4.3) into (4.2) leads to

$$L(\frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1}) = \mathcal{F}_{t_0}^{-1} T(\epsilon, \omega_0) \mathcal{F}_{t_0}$$
(4.4)

$$L(\frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1})^{-1} = \mathcal{F}_{t_0}^{-1} T(\epsilon, \omega_0)^{-1} \mathcal{F}_{t_0}$$
(4.5)

after some rearranging. This indicates that

$$\tilde{L}^{-1} = \mathcal{F}_{t_0}^{-1} T(\epsilon, \omega_0)^{-1} \mathcal{F}_{t_0}|_{\epsilon = 0 \to 1}$$
(4.6)

can be used in place of (2.33) as the conjugate approximation of L^{-1} . For those cases satisfying (4.2),

$$T_0^{-1} = T^{-1}(\epsilon, \omega_0)|_{\epsilon \to 0}$$

= $L(i\omega_0)^{-1}$. (4.7)

so that $T_0^{-1}f$ can be interpreted as the time-harmonic response of L to f at the frequency ν , where $\omega_0=2\pi\nu$. At a given frequency, the perturbational expansion about $\epsilon=0$ itself can be interpreted as a transient departure, on the t_1 (slow) time scale, from the time harmonic solution at $\nu=\omega_0/2\pi$. The only inversion required to obtain the Ω_j operators in (2.61) is T_0^{-1} , so that obtaining the Ω_j 's as a function of ω_0 reduces to time-harmonic re-analysis. A practical computational approximation is to restrict the range of ν values to a given frequency window of interest for the particular problem (2.1). At least one case satisfying (4.2) is that for which (2.1) is a set of linear coupled ordinary differential equations in time with constant coefficients, L then is a polynomial in the time derivative operator.

4.1.1 Linear Coupled O.D.E. Systems with Constant Coefficients

The ordinary differential equation setting is generic but at the same time well-rooted in concrete applications. This setting encompasses many useful classes of models, with examples arising from finite element methods (FEMs) and large linear electronic circuit response. Additionally, this setting is sufficiently specific in scope as to allow the explicit construction of the conjugate approximation results in terms of generic coefficient matrices for the differential equations. A summary of these results is given by the following theorem, whose proof is deferred to Appendix E.

Theorem 9 Let the system operator L for the Jth order set of ordinary differential equations (2.1) be denoted by

$$L = \sum_{j=0}^{J} \mathcal{L}_j \frac{\partial^j}{\partial t^j},\tag{4.8}$$

where the \mathcal{L}_j coefficients are constant, square matrices each of the same size. Applying the biscale perturbation of (4.3) to (4.8) leads to (2.34) for

$$T_j = \hat{T}_j(\omega_0) \frac{\partial^j}{\partial t_1^{\ j}} \tag{4.9}$$

$$\widehat{T}_k(\omega_0) = \sum_{m=k}^J \binom{m}{k} (i\omega_0)^{m-k} \mathcal{L}_m, \tag{4.10}$$

where the binomial coefficients are

$$\begin{pmatrix} m \\ k \end{pmatrix} = \frac{m!}{k!(m-k)!}.$$
 (4.11)

The conjugate approximation continuation (2.50) reduces to

$$T(\epsilon, \omega_0)^{-1} \approx \sum_{j=0}^{M} \epsilon^j \widehat{\Psi}_j(\omega_0) \frac{\partial^j}{\partial t_1^j},$$
 (4.12)

where the component matrices $\widehat{\Psi}_j$ are recursively given by

$$\widehat{\Psi}_{j} = H_{0j}\widehat{T}_{0}^{-1} - \sum_{k=1}^{J} H_{jk}\widehat{T}_{0}^{-1}\widehat{T}_{k}\widehat{\Psi}_{j-k}, \tag{4.13}$$

the ω_0 dependence being implied. The H_{jk} 's are defined by (2.38).

The conjugate approximation to L^{-1} given by (4.6) reduces to

$$\widetilde{L}^{-1} = \mathcal{F}_{t_0}^{-1} \left[\sum_{j=0}^{M} \widehat{\Psi}_j(\omega_0) \frac{\partial^j}{\partial t_1^j} \right] \mathcal{F}_{t_0}. \tag{4.14}$$

Note that (4.9) and (4.10) produce

$$\hat{T}_{J} = \mathcal{L}_{J}$$

$$\hat{T}_{0} = \sum_{m=0}^{J} (i\omega_{0})^{m} \mathcal{L}_{m}$$

$$= T_{0}$$
(4.15)

as important special cases. The bulk of the work in obtaining \tilde{L}^{-1} is in computing the time harmonic response \hat{T}_0^{-1} for values of ω_0 corresponding to the chosen frequency window.

4.2 Alternative ODE-Model Methods for Reduced Basis

In the case of reduced basis model reduction, an alternative variant of the ordinary differential equation biscale method of Section 4.1.1 serves as a precursor to and a generalization of the force derivative method. For $(I - L^I L)L^{-1} = L^{-1} - L^I$ in (2.4), an alternative form for (2.32) is

$$L^{-1} \approx \Lambda(\epsilon)|_{\epsilon} = 0 \to 1 \tag{4.17}$$

for

$$\Lambda(\epsilon) = L^{I^*} + [L^{-1} - L^{I^*}](\epsilon). \tag{4.18}$$

In this case, for which the ϵ -continuation of the conjugate approximation is extended to include the *entire* residual term $L^{-1} - L^{I^*}$, one gets

$$\Lambda(\epsilon) = \Phi_{d}(\Phi_{r}^{\dagger}L\Phi_{d})^{-1}\Phi_{r}^{\dagger} + \left\{ L(\frac{\partial}{\partial t_{0}} + \epsilon \frac{\partial}{\partial t_{1}})^{-1} - \Phi_{d}[\Phi_{r}^{\dagger}L(\frac{\partial}{\partial t_{0}} + \epsilon \frac{\partial}{\partial t_{1}})\Phi_{d}]^{-1}\Phi_{r}^{\dagger} \right\}$$

$$= \Phi_{d}(\Phi_{r}^{\dagger}L\Phi_{d})^{-1}\Phi_{r}^{\dagger} + \mathcal{F}_{t_{0}}^{-1} \left\{ T(\epsilon, \omega_{0})^{-1} - \Phi_{d}[\Phi_{r}^{\dagger}T(\epsilon, \omega_{0})\Phi_{d}]^{-1}\Phi_{r}^{\dagger} \right\} \mathcal{F}_{t_{0}}. \tag{4.19}$$

when using reduced basis version (3.14) of L^{I^*} , (4.4), and (4.5). If Φ_r and Φ_d are independent of ϵ and ω_0 , then Lemma 5 of Appendix E can be used with $\tau \to t_1$, $\hat{\Omega}_j \to \hat{\psi}_j$, and $\hat{T}_j \to \Phi_r^{\dagger} \hat{T}_j(\omega_0) \Phi_d$ from (2.34), (4.9), and $T(\epsilon) \to \Phi_r^{\dagger} T(\epsilon, \omega_0) \Phi_d$. This results in

$$[\Phi_r^{\dagger} T(\epsilon, \omega_0) \Phi_d]^{-1} \approx \sum_{i=0}^M \epsilon^j \hat{\psi}_j(\omega_0) \frac{\partial^j}{\partial t_1^{j}}, \tag{4.20}$$

where the component matrices $\hat{\psi}_j$ are recursively given by

$$\hat{\psi}_{j} = H_{0j}(\Phi_{r}^{\dagger} \hat{T}_{0} \Phi_{d})^{-1} - \left[\sum_{k=1}^{J} H_{jk}(\Phi_{r}^{\dagger} \hat{T}_{0} \Phi_{d})^{-1} (\Phi_{r}^{\dagger} \hat{T}_{k} \Phi_{d}) \hat{\psi}_{j-k} \right].$$
(4.21)

the ω_0 dependence is implied. Substituting (4.12) and (4.20) into (4.19) and the results into (4.17) leads to

$$L^{-1} \approx \Phi_d(\Phi_r^{\dagger}L\Phi_d)^{-1}\Phi_r^{\dagger} + \mathcal{F}_{t_0}^{-1} \left\{ \sum_{j=0}^{M} \left[\widehat{\Psi}_j(\omega_0) - \Phi_d \widehat{\psi}_j(\omega_0) \Phi_r^{\dagger} \right] \frac{\partial^j}{\partial t_1^{j}} \right\} \mathcal{F}_{t_0}$$

$$(4.22)$$

as a reduced basis hybrid method for sets of coupled ordinary differential equations, where the $\hat{\Psi}_j$'s are recursively given by (4.13).

4.2.1 Tunable Force Derivative and Generalized Lanczos Methods

One can generate a systematic approximation to the reduced basis hybrid method just developed by expanding

$$[\widehat{\Psi}_{j}(\omega_{0}) - \Phi_{d}\widehat{\psi}_{j}(\omega_{0})\Phi_{r}^{\dagger}] = \sum_{k=0}^{\infty} \frac{(\omega_{0} - \omega^{*})^{k}}{k!} \left\{ \frac{\partial [\widehat{\Psi}_{j} - \Phi_{d}\widehat{\psi}_{j}\Phi_{r}^{\dagger}]^{k}}{\partial \omega_{0}^{k}} \right\}_{\omega_{0} \to \omega^{*}}$$

about the value ω^* as a Taylor series, assuming an analytic dependence on ω_0 . If only the first term in the expansion is kept, one gets

$$\mathcal{F}_{t_0}^{-1} \left\{ \sum_{j=0}^{M} \left[\hat{\Psi}_j(\omega_0) - \Phi_d \hat{\psi}_j(\omega_0) \Phi_r^{\dagger} \right] \frac{\partial^j}{\partial t_1^{j}} \right\} \mathcal{F}_{t_0}$$

$$\approx \mathcal{F}_{t_0}^{-1} \left\{ \sum_{j=0}^{M} \left[\hat{\Psi}_j(\omega^*) - \Phi_d \hat{\psi}_j(\omega^*) \Phi_r^{\dagger} \right] \frac{\partial^j}{\partial t_1^{j}} \right\} \mathcal{F}_{t_0}$$

$$= \left\{ \sum_{j=0}^{M} \left[\hat{\Psi}_j(\omega^*) - \Phi_d \hat{\psi}_j(\omega^*) \Phi_r^{\dagger} \right] \frac{\partial^j}{\partial t_1^{j}} \right\} \mathcal{F}_{t_0}^{-1} \mathcal{F}_{t_0}$$

$$= \sum_{j=0}^{M} \left[\hat{\Psi}_j(\omega^*) - \Phi_d \hat{\psi}_j(\omega^*) \Phi_r^{\dagger} \right] \frac{\partial^j}{\partial t_1^{j}}$$

on the right-hand side of (4.22), so that

$$L^{-1} \approx \Phi_d(\Phi_r^{\dagger} L \Phi_d)^{-1} \Phi_r^{\dagger} + \sum_{i=0}^M [\hat{\Psi}_j(\omega^*) - \Phi_d \hat{\psi}_j(\omega^*) \Phi_r^{\dagger}] \frac{\partial^j}{\partial t_1^{j}}$$
(4.23)

results as the zeroth-order approximation to (4.22). It is proven later that the conventional force derivative method results from the $\omega^* \to 0$ subcase of (4.23), so that (4.23) represents a tunable generalization of the force derivative method.

Taking the above Taylor expansion in (4.19) leads to

$$\Lambda(\epsilon) = \Phi_d(\Phi_r^{\dagger} L \Phi_d)^{-1} \Phi_r^{\dagger} + \left\{ T(\epsilon, \omega^*)^{-1} - \Phi_d[\Phi_r^{\dagger} T(\epsilon, \omega^*) \Phi_d]^{-1} \Phi_r^{\dagger} \right\}$$
(4.24)

when keeping the first expansion-term only and canceling the Fourier transform with its inverse. The generalized Lanczos reduced basis method is based on the idea of finding Φ_d such that

$$\Lambda(\epsilon) = \Phi_d(\Phi_r^{\dagger} L \Phi_d)^{-1} \Phi_r^{\dagger} + \mathcal{O}(\epsilon^k)$$
(4.25)

for (4.24) for some chosen k > 0. For such a choice of Φ_d , only the $\Phi_d(\Phi_r^{\dagger}L\Phi_d)^{-1}\Phi_r^{\dagger}$ term needs to be kept in (4.23). Such a Φ_d can be constructed if one assumes that the admissible f's to be considered for (2.1) are to be taken exclusively from the set V, where $f \in V$ implies

$$f = Fg(t) (4.26)$$

for some g. The matrix F common to all of the f's is time-independent, and g is a time-dependent vector. In mechanics for example, (4.26) represents a superposition of static loads (columns of F) using time-varying coefficients (components of g). Choose the *block* columns of Φ_d as $\widehat{\Psi}_j(\omega^*)F$ in the left-to-right sequence $j=0,1,\ldots,k-1$, so that

$$\Phi_d(\omega^*) = \left(\hat{\Psi}_0(\omega^*) F \quad \hat{\Psi}_1(\omega^*) F \quad \cdots \quad \hat{\Psi}_{k-1}(\omega^*) F \right). \tag{4.27}$$

where the $\hat{\Psi}_j$'s are given by (4.13). The number of columns of F (and correspondingly, components of g) should be small compared to the size of (4.8), so that the number of columns of Φ_d , is small compared to

the number of rows of Φ_d . Taking $M \to k-1$ and $\omega_0 \to \omega^*$ in (4.12), applying the result to (4.26), and then substituting Φ_d for the right-hand side of (4.27) leads to

$$T(\epsilon, \omega^*)^{-1} f = \sum_{j=0}^{k-1} [\widehat{\Psi}_j(\omega^*) F] \epsilon^j \frac{\partial^j g}{\partial t_1^j} + \mathcal{O}(\epsilon^k)$$

$$= \Phi_d \begin{pmatrix} g \\ \epsilon \frac{\partial g}{\partial t_1} \\ \vdots \\ \epsilon^{k-1} \frac{\partial^{k-1} g}{\partial t_1^{k-1}} \end{pmatrix} + \mathcal{O}(\epsilon^k)$$

$$= \Phi_d h(\epsilon) + \mathcal{O}(\epsilon^k)$$

for $h(\epsilon)$ defined with block rows $\epsilon^j \partial^j g / \partial t_1^j$ in the top-to-bottom sequence $j = 0, 1, \dots, k-1$. Using this in

$$\begin{split} & \Phi_{d}[\Phi_{r}^{\dagger}T(\epsilon,\omega^{*})\Phi_{d}]^{-1}\Phi_{r}^{\dagger}f \\ & = \Phi_{d}[\Phi_{r}^{\dagger}T(\epsilon,\omega^{*})\Phi_{d}]^{-1}\Phi_{r}^{\dagger}T(\epsilon,\omega^{*})T(\epsilon,\omega^{*})^{-1}f + \mathcal{O}(\epsilon^{k}) \\ & = \Phi_{d}[\Phi_{r}^{\dagger}T(\epsilon,\omega^{*})\Phi_{d}]^{-1}\Phi_{r}^{\dagger}T(\epsilon,\omega^{*})\Phi_{d}h(\epsilon) + \mathcal{O}(\epsilon^{k}) \\ & = \Phi_{d}h(\epsilon) + \mathcal{O}(\epsilon^{k}) \\ & = T(\epsilon,\omega^{*})^{-1}f + \mathcal{O}(\epsilon^{k}) \end{split}$$

shows that (4.24) reduces to (4.25) for the choice of (4.27) for Φ_d . For first or second order (J=1 or 2) cases, this resembles the method of Häggblad and Eriksson [29]. The span of the columns of Φ_d , for Φ_d given by (4.27), will later be shown to reduce to a conventional Krylov subspace under special circumstances. In such cases, this becomes the conventional Lanczos method, with proper normalization of Φ_d 's columns.

4.3 Conventional Force Derivative Lanczos Submethods

For the linear dynamic mechanics class of finite-element models for which the force-derivative and Lanczos methods were originally developed, the ordinary differential equations are second order with real, constant, symmetric matrix coefficients. For the symmetric case, $\Phi_d = \Phi_r = \Phi$ is reasonable. The second-order representation (3.2) of (2.1) is given in terms of (4.8) for J=2 as

$$\mathcal{L}_0 = K \tag{4.28}$$

$$\mathcal{L}_1 = C \tag{4.29}$$

$$\mathcal{L}_2 = M. \tag{4.30}$$

where u(t) and f(t) of (2.1) are interpreted as the displacement response and applied loads, respectively. For an equivalent first-order (or state) representation [38, p. 12], L is given by (4.8) for J = 1 and

$$\mathcal{L}_1 = \begin{pmatrix} 0 & M \\ M & C \end{pmatrix} \tag{4.31}$$

$$\mathcal{L}_0 = \begin{pmatrix} -M & 0 \\ 0 & K \end{pmatrix}. \tag{4.32}$$

where the \mathcal{L}_0 and \mathcal{L}_1 matrices are constant, real, and symmetric since this is true for M, C, and K, and where

$$f \rightarrow \begin{pmatrix} 0 \\ f \end{pmatrix} \tag{4.33}$$

$$u \rightarrow \begin{pmatrix} \frac{du}{dt} \\ u \end{pmatrix} \tag{4.34}$$

are used in (2.1). The development that follows will use the second-order representation.

Equation (4.10) with $\omega_0 \to \omega^*$ reduces to

$$\hat{T}_0 = -\omega^{*2}M + i\omega^*C + K \tag{4.35}$$

$$\hat{T}_1 = 2i\omega^* M + \hat{C} \tag{4.36}$$

$$\hat{T}_2 = M \tag{4.37}$$

when using (4.28) through (4.30). The reduced basis versions of these coefficients become

$$\Phi^T \hat{T}_0 \Phi = -\omega^{*2} I + i\omega^* \beta + \Upsilon^2 \tag{4.38}$$

$$\Phi^T \hat{T}_1 \Phi = 2i\omega^* I + \beta \tag{4.39}$$

$$\Phi^T \hat{T}_2 \Phi = I \tag{4.40}$$

when using (3.20), (3.15), and (3.21). The $\hat{\psi}_i$ component matrices are recursively given by (4.21), which reduces to

$$\widehat{\psi}_0 = (\Phi^T \widehat{T}_0 \Phi)^{-1} \tag{4.41}$$

$$\hat{\psi}_1 = -(\Phi^T \hat{T}_0 \Phi)^{-1} (\Phi^T \hat{T}_1 \Phi) (\Phi^T \hat{T}_0 \Phi)^{-1}$$
(4.42)

$$\hat{\psi}_{m} = -(\Phi^{T} \hat{T}_{0} \Phi)^{-1} \left[(\Phi^{T} \hat{T}_{1} \Phi) \hat{\psi}_{m-1} + (\Phi^{T} \hat{T}_{2} \Phi) \hat{\psi}_{m-2} \right], \tag{4.43}$$

for $m \geq 2$. The $\widehat{\Psi}_j$ component matrices are recursively given by (4.13), which reduces to

$$\hat{\Psi}_0 = \hat{T}_0^{-1} \tag{4.44}$$

$$\hat{\Psi}_1 = -\hat{T}_0^{-1} \hat{T}_1 \hat{T}_0^{-1} \tag{4.45}$$

$$\hat{\Psi}_1 = -\hat{T}_0^{-1}\hat{T}_1\hat{T}_0^{-1} \tag{4.45}$$

$$\hat{\Psi}_m = -\hat{T}_0^{-1} \left[\hat{T}_1 \hat{\Psi}_{m-1} + \hat{T}_2 \hat{\Psi}_{m-2} \right]$$
(4.46)

for $m \geq 2$.

4.3.1 Force Derivative as a Submethod

The force-derivative method corresponds to the limiting subcase of $\omega^* \to 0$, so that in the second-orderrepresentation (4.35) through (4.37) reduce to

$$\hat{T}_0 = K \tag{4.47}$$

$$\hat{T}_1 = C$$
 (4.48)
 $\hat{T}_2 = M$. (4.49)

$$\hat{T}_2 = M. \tag{4.49}$$

The reduced basis versions of these coefficients (4.38) through (4.40) become

$$\Phi^T \hat{T}_0 \Phi = \Upsilon^2 \tag{4.50}$$

$$\Phi^T \hat{T}_1 \Phi = \beta \tag{4.51}$$

$$\Phi^T \hat{T}_2 \Phi = I. \tag{4.52}$$

The ψ_j component matrices of (4.41) through (4.43) reduce to

30

$$\hat{\psi}_0 = \Upsilon^{-2}$$
 (4.53)
 $\hat{\psi}_1 = -\Upsilon^{-2}\beta\Upsilon^{-2}$ (4.54)

$$\hat{\psi}_1 = -\Upsilon^{-2}\beta\Upsilon^{-2} \tag{4.54}$$

$$\hat{\psi}_m = -\Upsilon^{-2} \left[\beta \hat{\psi}_{m-1} + \hat{\psi}_{m-2} \right] \tag{4.55}$$

for $m \ge 2$, when using (4.50) through (4.52). The Ψ_i of (4.44) through (4.46) reduce to

$$\hat{\Psi}_0 = K^{-1} \tag{4.56}$$

$$\hat{\Psi}_1 = -K^{-1}CK^{-1} \tag{4.57}$$

$$\hat{\Psi}_m = -K^{-1} \left[C \hat{\Psi}_{m-1} + M \hat{\Psi}_{m-2} \right]$$
 (4.58)

for m > 2, when using (4.47) through (4.49). Taking $\omega^* \to 0$ is somewhat of a contradiction in the context of t_0 as the fast variable, for which ω_0 (and hence ω^*) is associated with "higher" frequencies. However, only the t_1 (slow) time scale remains (take $\omega^* \to 0$ and $\epsilon \to 1$ in (4.3)), suggesting $t_1 \to t$.

Using the first three terms of (4.53) through (4.55), the first three terms of (4.56) through (4.58), $\Upsilon^{-2} \to \Omega^{-2}, \ \beta \to \Lambda, \ \omega^* \to 0$, and $t_1 \to t$ for the slow time all in (4.23) reproduces (38) of Ref. [38, p. 29]. (The Υ^{-2} and β substitutions account for notational discrepencies between Ref. [38] and this report.) For the case of an arbitrary number of terms, taking $t_1 \to t$ and $\omega^* \to 0$ in (4.23), substituting this result for L^{-1} into L^{-1} f (from (2.1)), and then using the notational associations

$$\widehat{\phi} \longleftrightarrow \Phi$$
(4.59)

$$\hat{q} \longleftrightarrow (\Phi^T L \Phi)^{-1} \Phi^T f \tag{4.60}$$

$$Q^{(j)} \longleftrightarrow \frac{\partial^j}{\partial t_1^{\ j}} f \text{ for } j \ge 0$$
 (4.61)

$$A_{1,j} \longleftrightarrow \hat{\psi}_j \text{ for } j \ge 0$$
 (4.62)

$$A_{1,j} \longleftrightarrow \hat{\psi}_j \text{ for } j \ge 0$$

$$B_{1,j} \longleftrightarrow \hat{\Psi}_j \text{ for } j \ge 0$$

$$(4.62)$$

reproduces the conventional force derivative results (39) of Ref. [38, p. 30]. Proof of this essentially hinges on proving the correspondence between the ψ_j and Ψ_j coefficients of (4.53) through (4.58) of this report with the $A_{1,j}$ and $B_{1,j}$ coefficients of Ref. [38, p. 30] and [59, p. 716]. To show this, the equations given by both Ref. [38, p. 30], and by (A8), (A9), (A16), and (A17) of Ref. [59, p. 716], for the $A_{1,j}$ and $B_{1,j}$ coefficients are reproduced here as

$$A_{1,j} = -\Omega^{-2} \Lambda A_{1,j+1} - \Omega^{-2} A_{2,j-1} \text{ for } j \ge 1$$
(4.64)

$$A_{2,j} = A_{1,j-1} \text{ for } j \ge 1$$
 (4.65)

$$A_{1.0} = \Omega^{-2} \tag{4.66}$$

$$A_{2.0} = 0 (4.67)$$

and

$$B_{1,j} = -K^{-1}CB_{1,j-1} - K^{-1}MB_{2,j-1} \text{ for } j \ge 1$$
 (4.68)

$$B_{2,j} = B_{1,j-1} \text{ for } j \ge 1$$
 (4.69)
 $B_{1,0} = K^{-1}$ (4.70)

$$B_{1.0} = K^{-1} (4.70)$$

$$B_{2,0} = 0. (4.71)$$

respectively. (The notation Ω^{-2} and Λ of Ref. [59] corresponds to Υ^{-2} and β of this report, respectively. The "hats" on $\hat{\Omega}^{-2}$ and $\hat{\Lambda}$ of Ref. [38] have been "dropped" in favor of the notation of Ref. [59].) It is readily verified that $\Omega^{-2} \to \Upsilon^{-2}$ and $\Lambda \to \beta$ in (4.66), (4.67), and the i=1 case of (4.64) lead to

$$A_{1,1} = -\Upsilon^{-2}\beta\Upsilon^{-2},\tag{4.72}$$

and that (4.70), (4.71), and the j = 1 case of (4.68) lead to

$$B_{1,1} = -K^{-1}CK^{-1}. (4.73)$$

Equations (4.53), (4.54), and (4.62) are in agreement with $\Omega^{-2} \to \Upsilon^{-2}$ in (4.66) and (4.72), and equations (4.56), (4.57), and (4.63) are in agreement with (4.70) and (4.73). Equations (4.62) and (4.63) are verified for j=0,1. Taking $j \to j'-1$ and dropping the prime, equation (4.65) leads to

$$A_{2,j-1} = A_{1,j-2}$$
 for $j \ge 2$.

and (4.69) leads to

$$B_{2,j-1} = B_{1,j-2}$$
 for $j \ge 2$.

Substituting these into (4.64) and (4.68) leads to

$$A_{1,j} = -\Upsilon^{-2}\beta A_{1,j-1} - \Upsilon^{-2}A_{1,j-2} \text{ for } j \ge 2$$
(4.74)

and

$$B_{1,j} = -K^{-1}CB_{1,j-1} - K^{-1}MB_{1,j-2} \text{ for } j \ge 2,$$
(4.75)

respectively, when using $\Omega^{-2} \to \Upsilon^{-2}$ and $\Lambda \to \beta$. Substituting (4.62) into (4.74) and (4.63) into (4.75) leads to (4.55) and (4.58), respectively. Equations (4.62) and (4.63) are verified for $j \ge 2$ as well. Taking $t_1 \to t$ and $\omega^* \to 0$ into (4.23), substituting this result for L^{-1} into $L^{-1}f$, and then using (4.53) through (4.58) in the results is collectively equivalent to the conventional force derivative results of Ref. [38, p. 30] for second-order formulated systems.

4.3.2 Lanczos as a Submethod

In the limiting subcase $\omega^* \to 0$, (4.13) reduces to (4.56) through (4.58) for the $\hat{\Psi}_i$'s defining Φ in (4.27). If one takes C = 0 in (4.56) through (4.58), they further reduce to

$$\hat{\Psi}_0 = K^{-1} \tag{4.76}$$

$$\hat{\Psi}_{2j-1} = 0 \text{ for } j \ge 1$$

$$\hat{\Psi}_{2j} = (-K^{-1}M)^{j}K^{-1} \text{ for } j \ge 1,$$
(4.78)

$$\hat{\Psi}_{2j} = (-K^{-1}M)^j K^{-1} \text{ for } j \ge 1,$$
 (4.78)

so that (4.27) reduces to

$$\Phi = \begin{pmatrix} K^{-1}F & (-K^{-1}M)K^{-1}F & \cdots & (-K^{-1}M)^{\ell}K^{-1}F \end{pmatrix}$$
 (4.79)

after eliminating the zero columns arising from the $\hat{\Psi}_j$'s of odd j, where $\ell=(k-1)/2$ for even k-1 and $\ell=(k-2)/2$ for odd k-1. Except for the (irrelevant) alternating sign with each power of $-K^{-1}M$, the columns of Φ in (4.79) are seen to form a *block* version of the Krylov sequence (Ref. [24, p. 566]) traditionally associated with L specialized to J=2 in (4.8). The initial block $K^{-1}F$ of (4.79), whose columns are the static solutions to the loads of the columns of F, is the usual recommended initializing choice (Ref. [24, p. 568]) for the Krylov sequence in reduced basis applications. (The case for which F has just one column and F just one component results in the standard, "nonblock" version of the Krylov sequence.) The conventional Lanczos method uses a reduced basis consisting of the above Krylov sequence, which has been orthonormalized with respect to the mass matrix.

One might suspect that the C=0 assumption may hurt the Lanczos method's ability to handle general damping cases, and some evidence of this is found in the conclusions of Ref. [36]. In particular, the force-derivative method, which uses a finite set of the *nonzero-C'\hat{\Phi}_j*'s given by (4.56) through (4.58), efficiently and accurately handles the nonproportional damping case of Ref. [36], in contrast to the Lanczos method. Nevertheless, one possible advantage to the usual Krylov sequence (from the C=0 assumption) in conjunction with the orthonormalization process is that together they produce a *tridiagonal* reduced problem (see Nour-Omid and Clough (Ref. [24, pp. 567, 569]) or Golub and Van Loan (Ref. [60, p. 477])).

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Appendix A

A. PROOF OF THEOREM 2

The following lemmas are preliminary to proving theorem 2.

Lemma 1 Given operators P_d , P_r , and T, the operator $P_d(P_rTP_d)^IP_r$, when it exists, is an outer generalized inverse of T.

Proof: Substituting $P_d(P_rTP_d)^IP_r$ for A^I in A^IAA^I leads to

$$P_{d}(P_{r}TP_{d})^{I}P_{r}TP_{d}(P_{r}TP_{d})^{I}P_{r} = P_{d}(P_{r}TP_{d})^{I}(P_{r}TP_{d})(P_{r}TP_{d})^{I}P_{r}$$

= $P_{d}(P_{r}TP_{d})^{I}P_{r}$,

proving the lemma.

Lemma 2 Given a fixed linear operator T and two fixed linear, idempotent P_d and P_r , $P_dT^IP_r$ is unique for all T^I such that

$$P_d T^I T = P_d \tag{A.1}$$

$$TT^{I}P_{r} = P_{r} \tag{A.2}$$

are simultaneously true.

Proof: Suppose that there are two outer generalized inverses of T, label them T_1^I and T_2^I , each of which satisfied (A.1) and (A.2) simultaneously. They would obviously satisfy

$$P_d T_1{}^I T = P_d T_2{}^I T \tag{A.3}$$

$$TT_1{}^I P_r = TT_2{}^I P_r, (A.4)$$

and because they are outer generalized inverses of T, they would also satisfy

$$T_1^I T T_1^I = T_1^I T_2^I T T_2^I = T_2^I,$$

and hence

$$P_{d}T_{1}{}^{I}TT_{1}{}^{I}P_{r} = P_{d}T_{1}{}^{I}P_{r} \tag{A.5}$$

$$P_d T_2{}^I T T_2{}^I P_r = P_d T_2{}^I P_r. (A.6)$$

Substituting (A.4) into (A.5), and (A.3) into (A.6), leads to

$$P_d T_1^I T T_2^I P_r = P_d T_1^I P_r$$

 $P_d T_1^I T T_2^I P_r = P_d T_2^I P_r$,

respectively. These final two equations clearly show that $P_dT_1{}^IP_r=P_dT_2{}^IP_r$, and the lemma's proof is complete.

Lemma 3 Given two linear idempotent operators P and Π ,

$$P\Pi = \Pi \longrightarrow$$

$$\mathcal{R}(\Pi) \subseteq \mathcal{R}(P)$$

$$P\Pi = P \longrightarrow$$
(A.7)

$$\mathcal{R}(P) \subseteq \mathcal{R}(\Pi) . \tag{A.8}$$

Proof: If $t \in \mathcal{R}(\Pi)$ then $t = \Pi t = P\Pi t = Pt$ so that $t \in \mathcal{R}(P)$, proving (A.7). The relation $P\Pi = P$ implies $P(I - \Pi) = 0$, which implies $(I - P)(I - \Pi) = (I - \Pi)$, which in turn implies $\mathcal{R}(I - \Pi) \subseteq \mathcal{R}(I - P)$ by (A.7). This, in conjunction with $\mathcal{R}(I - \Pi) = \mathcal{N}(\Pi)$ and $\mathcal{R}(I - P) = \mathcal{N}(P)$, leads to $\mathcal{N}(\Pi) \subseteq \mathcal{N}(P)$. Using the fact that $A^C \subseteq B^C$ implies $B \subseteq A$ for generic A and B, $\mathcal{N}(\Pi)^C = \mathcal{R}(\Pi) - \{0\}$, and $\mathcal{N}(P)^C = \mathcal{R}(P) - \{0\}$ in the results leads to $\mathcal{R}(P) - \{0\} \subseteq \mathcal{R}(\Pi) - \{0\}$, where the superscript C denotes the (set) complement. The union of both sides of this result with $\{0\}$, along with $0 \in \mathcal{R}(\Pi)$ and $0 \in \mathcal{R}(P)$, leads to (A.8).

The proof of Theorem 2 itself is now given as follows.

- To show that L^{I^*} is an outer generalized inverse of L, use (2.10) to substitute P_rLP_d for L_{eff} in (2.11), and then apply Lemma 1, with $T \to L$, to the result.
- To prove (2.12), let $v \in \mathcal{N}(P_r L)$. One then has $(I L^{I^*} L)v = (I P_d L_{\epsilon ff}{}^I P_r L)v = v$ from (2.11) for idempotent $(I L^{I^*} L)$, so that $v \in \mathcal{R}(I L^{I^*} L)$, proving (2.12).
- The relation $L^{I*}LP_d = P_dL_{eff}^IP_rLP_d = P_dL_{eff}^IL_{eff} = P_d$ follows from (2.11), (2.10), and (2.13), proving that (2.16) follows from (2.13). The converse, that (2.13) follows from (2.16), is also clearly true.
- To prove (2.15) follows from (2.13), one first notes that application of (A.7) of Lemma 3, with $P \to P_d$ and $\Pi \to L^{I*}L$, to $P_dL^{I*}L = P_d^2L_{eff}^IP_rL = P_dL_{eff}^IP_rL = L^{I*}L$ leads to $\mathcal{R}(L^{I*}L) \subseteq \mathcal{R}(P_d)$. However, application of (A.7) of Lemma 3, with $P \to L^{I*}L$ and $\Pi \to P_d$, to (2.16) leads to $\mathcal{R}(P_d) \subseteq \mathcal{R}(L^{I*}L)$. Together these results prove $\mathcal{R}(L^{I*}L) = \mathcal{R}(P_d)$, which combines with $\mathcal{R}(L^{I*}L) = \mathcal{N}(I L^{I*}L)$ to prove (2.15).
- To prove (2.17) follows from (2.13), one starts with $[\mathcal{R}(P_d) \cap \mathcal{N}(P_rL)] \subseteq [\mathcal{R}(P_d) \cap \mathcal{R}(I-L^{I^*}L)] = [\mathcal{N}(I-L^{I^*}L) \cap \mathcal{R}(I-L^{I^*}L)] = \{0\}$, which follows from (2.12) and (2.15). Substituting this into $\mathcal{N}(L_{\epsilon ff}) = \{[\mathcal{R}(P_d) \cap \mathcal{N}(P_rL)] \cup \mathcal{N}(P_d)\}$, which follows from (2.10), leads to (2.17) upon using $0 \in \mathcal{N}(P_d)$.
- The relation $P_r L L^{I^*} = P_r L P_d L_{\epsilon ff}{}^I P_r = L_{\epsilon ff} L_{\epsilon ff}{}^I P_r = P_r$ follows from (2.11), (2.10), and (2.14), proving that (2.19) follows from (2.14). The converse, that (2.14) follows from (2.19), is also clearly true.
- To prove (2.18) follows from (2.14), one first notes that application of (A.8) of Lemma 3, with $P \to LL^{I^*}$ and $\Pi \to P_r$, to $LL^{I^*}P_r = LP_dL_{\epsilon ff}^IP_r^2 = LP_dL_{\epsilon ff}^IP_r = LL^{I^*}$ leads to $\mathcal{R}(LL^{I^*}) \subseteq \mathcal{R}(P_r)$. However, application of (A.8) of Lemma 3, with $P \to P_r$ and $\Pi \to LL^{I^*}$, to (2.19) leads to $\mathcal{R}(P_r) \subseteq \mathcal{R}(LL^{I^*})$. Together these results prove $\mathcal{R}(LL^{I^*}) = \mathcal{R}(P_r)$, which combines with $\mathcal{R}(LL^{I^*}) = \mathcal{N}(I LL^{I^*})$ to prove (2.18).
- To prove (2.20) follows from (2.14), first note that $P_rL(I-L^{I^*}L)=(P_r-P_rLL^{I^*})L=(P_r-P_r)L=0$ follows from (2.19), so that $\mathcal{R}(I-L^{I^*}L)\subseteq\mathcal{N}(P_rL)$. This result combines with (2.12) to prove (2.20).

- As $T \to L_{\epsilon ff}$ in (A.1) and (A.2) of Lemma 2 corresponds to (2.13) and (2.14), respectively, then (2.11) and Lemma 2 together show that L^{I^*} is unique when (2.13) and (2.14) are simultaneously satisfied.
- The relation $L^{I*}L = P_dL_{\epsilon ff}{}^IP_rL = P_dL_{\epsilon ff}{}^IP_rLP_d = P_dL_{\epsilon ff}{}^IL_{\epsilon ff} = P_d$ follows from (2.11), (2.21), (2.10), and (2.13), proving that (2.22) follows from (2.13) and (2.21).
- The relations (2.21) and (2.22) imply $0 = P_r L(I P_d) = P_r L(I L^{I*}L) = (P_r P_r LL^{I*})L$, so that $\mathcal{R}(L) \subseteq \mathcal{N}(P_r P_r LL^{I*})$. This proves (2.16), from which (2.13) follows.
- The relation $LL^{I^*} = LP_dL_{\epsilon ff}^IP_r = P_rLP_dL_{\epsilon ff}^IP_r = L_{\epsilon ff}L_{\epsilon ff}^IP_r = P_r$ follows from (2.11), (2.23), (2.10), and (2.14), proving that (2.24) follows from (2.14) and (2.23).
- The relations (2.23) and (2.24) imply $0 = (I P_r)LP_d = (I LL^{I^*})LP_d = L(P_d L^{I^*}LP_d)$, so that $\mathcal{R}(P_d L^{I^*}LP_d) \subseteq \mathcal{N}(L) = \{0\}$. This proves (2.19), from which (2.14) follows.

The proof of Theorem 2 is complete.

Appendix B

B. PROOF OF THEOREM 4

Equations (2.34), (2.35), (2.39), and (2.40) can be rewritten as

$$T(\epsilon) = \sum_{j=0}^{\infty} \epsilon^{j} H_{Jj} T_{j}$$
 (B.1)

$$\Gamma^{b}(\epsilon) = \sum_{j=0}^{\infty} \epsilon^{j} H_{Nj} \Gamma^{b}{}_{j}$$
 (B.2)

$$\Omega^{b}(\epsilon) = \sum_{j=0}^{\infty} \epsilon^{j} H_{Mj} \Omega^{b}{}_{j}, \tag{B.3}$$

respectively, where $b \to R$ or L, so that

$$T\Omega^{R} = \sum_{j=0}^{\infty} \epsilon^{j} \left[\sum_{k=0}^{j} H_{Jk} T_{k} H_{M,j-k} \Omega^{R}_{j-k} \right].$$

when taking $b \to R$ in (B.3), for example. This becomes

$$T\Omega^{R} = \sum_{j=0}^{\infty} \epsilon^{j} \left[\sum_{k=0}^{J} H_{jk} H_{M,j-k} T_{k} \Omega^{R}_{j-k} \right]$$
(B.4)

when using

$$\sum_{k=0}^{j} H_{Jk} A_{jk} = \sum_{k=0}^{\infty} H_{jk} H_{Jk} A_{jk}$$

$$= \sum_{k=0}^{J} H_{jk} A_{jk}$$
(B.5)

for generic A_{jk} . Similarly,

$$\Omega^{L}T = \sum_{i=0}^{\infty} \epsilon^{j} \left[\sum_{k=0}^{J} H_{jk} H_{M,j-k} \Omega^{L}_{j-k} T_{k} \right]$$
(B.6)

for $b \to L$ in (B.3) and $A_{jk} \to \Omega^L{}_{j-k}T_k$ in (B.5). For (B.4) and $b \to R$ in (B.2), one gets

$$T\Omega^{R} - \Gamma^{R} = \sum_{j=0}^{\infty} \epsilon^{j} \left[\left(\sum_{k=0}^{J} H_{jk} H_{M,j-k} T_{k} \Omega^{R}_{j-k} \right) - H_{Nj} \Gamma^{R}_{j} \right]$$
$$= \sum_{j=0}^{M} \epsilon^{j} \left[\left(\sum_{k=0}^{J} H_{jk} H_{M,j-k} T_{k} \Omega^{R}_{j-k} \right) - H_{Nj} \Gamma^{R}_{j} \right]$$

$$\begin{split} &+\sum_{j=M+1}^{\infty}\epsilon^{j}\bigg[\bigg(\sum_{k=0}^{J}H_{jk}H_{M,j-k}T_{k}\Omega^{R}{}_{j-k}\bigg)-H_{Nj}\Gamma^{R}{}_{j}\bigg]\\ &=&\sum_{j=0}^{M}\epsilon^{j}\bigg[\bigg(\sum_{k=0}^{J}H_{jk}T_{k}\Omega^{R}{}_{j-k}\bigg)-H_{Nj}\Gamma^{R}{}_{j}\bigg]\\ &+\sum_{j=M+1}^{\infty}\epsilon^{j}\bigg[\bigg(\sum_{k=0}^{J}H_{jk}H_{M,j-k}T_{k}\Omega^{R}{}_{j-k}\bigg)-H_{Nj}\Gamma^{R}{}_{j}\bigg]\\ &=&\sum_{j=0}^{M}\epsilon^{j}\bigg[\bigg(\sum_{k=0}^{J}H_{jk}T_{k}\Omega^{R}{}_{j-k}\bigg)-H_{Nj}\Gamma^{R}{}_{j}\bigg]\\ &+\sum_{j=M+1}^{\mathbf{Max}(N,M+J)}\epsilon^{j}\bigg[\bigg(\sum_{k=0}^{J}H_{jk}H_{M,j-k}T_{k}\Omega^{R}{}_{j-k}\bigg)-H_{Nj}\Gamma^{R}{}_{j}\bigg]. \end{split}$$

The step from the second to the third line uses $H_{M,j-k}=1$ for $j\leq M$. The last line results from

$$\left\{ \begin{array}{l} j > \operatorname{Max}(N, M+J) \text{ and } \\ 0 \leq k \leq J \end{array} \right\} \quad \rightarrow \quad \left\{ \begin{array}{l} H_{M,j-k} = 0 \text{ and } \\ H_{Nj} = 0 \end{array} \right\}.$$

which follows from $\{j > \text{Max}(N, M + J)\} \rightarrow \{j > M + J \text{ and } j > N\},\$

so that $H_{Nj}=0$ and j-k>M+J-k; but $\{0\leq k\leq J\}\to\{M+J-k\geq M\}$, so that j-k>M and hence $H_{M,j-k}=0$.

Finally, the previous result establishes the equivalence of

$$\sum_{j=0}^{M} \epsilon^{j} \left[\left(\sum_{k=0}^{J} H_{jk} T_{k} \Omega^{R}_{j-k} \right) - H_{Nj} \Gamma^{R}_{j} \right] = 0$$

and (2.41). Solving this for $T_0\Omega^R_j$ leads to (2.36). The proof of (2.37) and (2.42) from (B.6) is essentially the same except that $\Omega^L_{j-k}T_k$ and Γ^L_j replace $T_k\Omega^R_{j-k}$ and Γ^R_j , respectively.

Appendix C

C. PROOF OF THEOREM 5

One can prove $\Omega^R_{\ j} = \Omega^L_{\ j}$ for each $j \geq 0$ by induction, where the initial case for j = 0, $\Omega^R_{\ 0} = \Omega^L_{\ 0} = A$, follows directly from (2.45) and (2.46). The strategy is to first *assume* that

$$\Omega^L_{j-k} = \Omega^R_{j-k} \tag{C.1}$$

for $1 \le k \le \min(J, j)$ and then prove that (2.45) and (2.46) subsequently lead to $\Omega^R_j = \Omega^L_j$. Substituting (C.1) into the left-hand side of (2.46) with $m \to j-k$ leads to

$$\Omega^{R}{}_{j-k} = H_{0,j-k}A - \sum_{\ell=1}^{J} H_{j-k,\ell} \Omega^{L}{}_{j-(\ell+k)} T_{\ell} A.$$

Substituting this result into the right-hand side of (2.45) with $m \rightarrow j$ leads to

$$\begin{split} \Omega^{R_{j}} &= H_{0j}A - \sum_{k=1}^{J} H_{jk}AT_{k}\Omega^{R}_{j-k} \\ &= H_{0j}A - \sum_{k=1}^{J} H_{jk}AT_{k} \bigg[H_{0,j-k}A - \sum_{\ell=1}^{J} H_{j-k,\ell}\Omega^{L}_{j-(\ell+k)}T_{\ell}A \bigg] \\ &= H_{0j}A - \sum_{k=1}^{J} H_{jk}H_{0,j-k}AT_{k}A \\ &+ \sum_{k=1}^{J} \sum_{\ell=1}^{J} H_{jk}H_{j-k,\ell}AT_{k}\Omega^{L}_{j-(\ell+k)}T_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell}H_{0,j-\ell}AT_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell} \bigg[H_{0,j-\ell}A - \sum_{k=1}^{J} H_{j-\ell,k}AT_{k}\Omega^{L}_{j-(\ell+k)} \bigg] T_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell} \bigg[H_{0,j-\ell}A - \sum_{k=1}^{J} H_{j-\ell,k}AT_{k}\Omega^{R}_{(j-\ell)-k} \bigg] T_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell}\Omega^{R}_{j-\ell}T_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell}\Omega^{R}_{j-\ell}T_{\ell}A \\ &= H_{0j}A - \sum_{\ell=1}^{J} H_{j\ell}\Omega^{L}_{j-\ell}T_{\ell}A \\ &= \Omega^{L}_{j} \end{split}$$

when using $H_{jk}H_{j-k,\ell}=H_{j\ell}H_{j-\ell,k}$ (proof follows), $\Omega^L_{(j-\ell)-k}=\Omega^R_{(j-\ell)-k}$ by (C.1); (2.45) with $m\to j-\ell$, $\Omega^R_{j-\ell}=\Omega^L_{j-\ell}$ by (C.1) since $1\le\ell\le \min(J,j)$ in the summation for ℓ , and (2.46) with $m\to j$, respectively. The proof reduces to that of proving that $H_{jk}H_{j-k,\ell}=H_{j\ell}H_{j-\ell,k}$ for $1\le k\le \min(J,j)$ and $1\le\ell\le \min(J,j)$.

The general property

$$H_{i\pm k, i\pm k} = H_{ij}$$

for all integers i, j, and k, leads to

$$H_{j-k,\ell} = H_{j,\ell+k}$$

$$= H_{j-\ell,k}.$$
(C.2)

One can prove

$$H_{ik}H_{i,\ell+k} = H_{i,\ell+k} \tag{C.3}$$

as follows: one has either $H_{j,\ell+k}=0$ or $H_{j,\ell+k}=1$. An assumption of $H_{j,\ell+k}=0$ implies that $H_{jk}H_{j,\ell+k}=0$. An assumption of $H_{j,\ell+k}=1$ implies $k+\ell \leq j$, which in turn implies $k \leq j$ because all values of ℓ are positive, so that $H_{jk}=1$ and $H_{jk}H_{j,\ell+k}=1$. As ℓ and k have exactly the same range of values, the proof of the relation

$$H_{j\ell}H_{j,\ell+k} = H_{j,\ell+k} \tag{C.4}$$

is essentially the same as that of (C.3). In fact, (C.4) is just a relabeling of (C.3). Substitute $H_{j-\ell,k}$ from (C.2) into the left-hand side of (C.4), substitute $H_{j-k,\ell}$ from (C.2) into the left-hand side of (C.3), and equate the results (the right-hand sides of each are equal) to prove $H_{jk}H_{j-k,\ell}=H_{j\ell}H_{j-\ell,k}$.

Appendix D

D. PROOF OF THEOREMS 6 and 7

Proof of Theorem 6: The proof of (3.29) is given by

$$\begin{split} P_{r}\Phi_{r} &= \mathcal{P}^{-1}\Pi_{\alpha}\mathcal{P}\Phi_{r} \\ &= \mathcal{P}^{-1}\Pi_{\alpha}\tilde{\Phi}_{r} \\ &= \mathcal{P}^{-1}\begin{pmatrix} I_{mm} & 0 \\ \alpha & 0 \end{pmatrix}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ [\tilde{\Phi}_{r}]_{s} \end{pmatrix} \\ &= \mathcal{P}^{-1}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ \alpha[\tilde{\Phi}_{r}]_{m} \end{pmatrix} \\ &= \mathcal{P}^{-1}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ [\tilde{\Phi}_{r}]_{s} \end{pmatrix} \\ &= \mathcal{P}^{-1}\tilde{\Phi}_{r} \\ &= \Phi_{r}, \end{split}$$

using (3.35), (3.32), $\gamma \to \alpha$ in (3.33), (3.31), (3.34), (3.31) again, and (3.32) again, respectively. The preliminary result

$$\mathcal{P}^{-1}\tilde{L}\Pi_{\beta}\mathcal{P} = \mathcal{P}^{-1}\begin{pmatrix} \tilde{L}_{mm} & \tilde{L}_{ms} \\ \tilde{L}_{sm} & \tilde{L}_{ss} \end{pmatrix}\begin{pmatrix} I_{mm} & 0 \\ \beta & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\begin{pmatrix} \tilde{L}_{mm} + \tilde{L}_{ms}\beta & 0 \\ \tilde{L}_{sm} + \tilde{L}_{ss}\beta & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\begin{pmatrix} \tilde{L}_{mm} + \tilde{L}_{ms}\beta & 0 \\ \alpha[\tilde{L}_{mm} + \tilde{L}_{ms}\beta] & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\begin{pmatrix} L_{red} & 0 \\ \alpha L_{red} & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\begin{pmatrix} I_{mm} & 0 \\ \alpha & 0 \end{pmatrix}\begin{pmatrix} L_{red} & 0 \\ 0 & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\Pi_{\alpha}\begin{pmatrix} L_{red} & 0 \\ 0 & 0 \end{pmatrix}\mathcal{P}$$

$$= \mathcal{P}^{-1}\Pi_{\alpha}\Theta\mathcal{P}$$

follows from using (3.28) and $\gamma \to \beta$ in (3.33), $\tilde{L}_{sm} + \tilde{L}_{ss}\beta = \alpha[\tilde{L}_{mm} + \tilde{L}_{ms}\beta]$ from (3.36), (3.38), $\gamma \to \alpha$ in (3.33), and (3.40), respectively. Substituting $LP_d = \mathcal{P}^{-1}\tilde{L}\mathcal{P}\mathcal{P}^{-1}\Pi_\beta\mathcal{P} = \mathcal{P}^{-1}\tilde{L}\Pi_\beta\mathcal{P}$ from (3.27) and (3.37) into the previous result leads to

$$LP_d = \mathcal{P}^{-1} \Pi_{\alpha} \Theta \mathcal{P}. \tag{D.1}$$

Matrix multiplying (D.1) from the left by P_r and substituting $P_r \mathcal{P}^{-1}\Pi_o = \mathcal{P}^{-1}\Pi_o \mathcal{P} \mathcal{P}^{-1}\Pi_o = \mathcal{P}^{-1}\Pi_o^2 = \mathcal{P}^{-1}\Pi_o$, from (3.35) into the result leads to $LP_d = P_r LP_d$, which proves (2.23). This gives $LP_d = L_{eff}$, when using (2.10), which combines with (D.1) to give

$$L_{eff} = \mathcal{P}^{-1} \Pi_{o} \Theta \mathcal{P}. \tag{D.2}$$

The $L_{eff}{}^I$ of (3.39) is proven to be an outer generalized inverse of L_{eff} from (D.2) by $L_{eff}{}^I L_{eff} L_{eff}{}^I = \mathcal{P}^{-1}\Theta^I\Pi_{\circ}\Theta\Theta^I\mathcal{P} = \mathcal{P}^{-1}\Theta^I\Theta\Theta^I\mathcal{P} = \mathcal{P}^{-1}\Theta^I\mathcal{P} = L_{eff}{}^I$, where $\Theta^I\Pi_{\circ} = \Theta^I$ is easily verified from $\gamma \to \alpha$ in (3.33) and (3.41). The relation (2.13) is proven by $P_d L_{eff}{}^I L_{eff} = \mathcal{P}^{-1}\Pi_{\beta}\Theta^I\Pi_{\circ}\Theta\mathcal{P} = \mathcal{P}^{-1}\Pi_{\beta}\Theta^I\Theta\mathcal{P} = \mathcal{P}^{-1}\Pi_{\beta}\Pi_{\circ}\mathcal{P} = \mathcal{P}^{-1}\Pi_{\beta}\mathcal{P} = P_d$ when using $\Theta^I\Pi_{\circ} = \Theta^I$ again; $\Theta^I\Theta = \Pi_0$ from $\gamma \to 0$ in (3.33), and $\Pi_{\beta}\Pi_{0} = \Pi_{\beta}$. The relation (2.14) follows from $L_{eff}L_{eff}{}^I = \mathcal{P}^{-1}\Pi_{\circ}\Theta\Theta^I\mathcal{P} = \mathcal{P}^{-1}\Pi_{\circ}\Pi_{0}\mathcal{P} = \mathcal{P}^{-1}\Pi_{\circ}\mathcal{P} = P_d$. Finally, using $\Theta^I\Pi_{\circ} = \Theta^I$ again in $L^{I*} = P_d L_{eff}{}^I P_r = \mathcal{P}^{-1}\Pi_{\beta}\Theta^I\Pi_{\circ}\mathcal{P}$ proves (3.42).

Proof of Theorem 7: Matrix multiplying (D.1) on the right by $\mathcal{P}^{-1}([\tilde{\Phi}_d]_m^T 0)^T$, substituting for Θ from (3.40), substituting for $P_d\mathcal{P}^{-1} = \mathcal{P}^{-1}\Pi_\beta$ from (3.37), and then substituting Φ_d from (3.45) gives

$$\mathcal{P}^{-1}\Pi_{o}\left(\begin{array}{c}L_{red}[\tilde{\Phi}_{d}]_{m}\\0\end{array}\right) = L\mathcal{P}^{-1}\Pi_{\beta}\left(\begin{array}{c}[\tilde{\Phi}_{d}]_{m}\\0\end{array}\right)$$
$$= L\Phi_{d}.$$

Right matrix multiplying (3.44) by $([\tilde{\Phi}_r]_m^{-1} 0)$ gives

$$\mathcal{P}^{-1}\Pi_{\alpha} = \Phi_r \Big(\begin{bmatrix} \tilde{\Phi}_r \end{bmatrix}_m^{-1} = 0 \Big).$$

when using $([\tilde{\Phi}_r]_m^T 0)^T ([\tilde{\Phi}_r]_m^{-1} 0) = \Pi_0$ for $\gamma \to 0$ in (3.33), and $\Pi_{\phi} \Pi_0 = \Pi_{\phi}$. Substituting this for $\mathcal{P}^{-1}\Pi_{\phi}$ into the previous result and then matrix multiplying on the left by Φ_r^{-1} leads to

$$\Phi_r^{\dagger} L \Phi_d = (\Phi_r^{\dagger} \Phi_r) \left(\begin{bmatrix} \tilde{\Phi}_r \end{bmatrix}_m^{-1} & 0 \right) \begin{pmatrix} L_{red} [\tilde{\Phi}_d]_m \\ 0 \end{pmatrix}
= (\Phi_r^{\dagger} \Phi_r) [\tilde{\Phi}_r]_m^{-1} L_{red} [\tilde{\Phi}_d]_m.$$
(D.3)

Inverting (D.3) and matrix multiplying the result on the left by Φ_d gives

$$\begin{split} \Phi_{d}(\Phi_{r}^{\dagger}L\Phi_{d})^{-1} &= \Phi_{d}[\tilde{\Phi}_{d}]_{m}^{-1}L_{r\epsilon d}^{-1}[\tilde{\Phi}_{r}]_{m}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= \mathcal{P}^{-1}\Pi_{\beta}\begin{pmatrix} I_{mm} \\ 0 \end{pmatrix}L_{r\epsilon d}^{-1}[\tilde{\Phi}_{r}]_{m}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= \mathcal{P}^{-1}\Pi_{\beta}\begin{pmatrix} L_{r\epsilon d}^{-1}[\tilde{\Phi}_{r}]_{m} \\ 0 \end{pmatrix}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= \mathcal{P}^{-1}\Pi_{\beta}\begin{pmatrix} L_{r\epsilon d}^{-1} & 0 \\ 0 & 0 \end{pmatrix}\mathcal{P}\mathcal{P}^{-1}\begin{pmatrix} I_{mm} & 0 \\ \alpha & 0 \end{pmatrix}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ 0 \end{pmatrix}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= \mathcal{P}^{-1}\Pi_{\beta}\Theta^{I}\mathcal{P}\mathcal{P}^{-1}\Pi_{\alpha}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ 0 \end{pmatrix}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= L^{I*}_{sub}\mathcal{P}^{-1}\Pi_{\alpha}\begin{pmatrix} [\tilde{\Phi}_{r}]_{m} \\ 0 \end{pmatrix}(\Phi_{r}^{\dagger}\Phi_{r})^{-1} \\ &= L^{I*}_{sub}\Phi_{r}(\Phi_{r}^{\dagger}\Phi_{r})^{-1}, \end{split}$$

when using

$$\Phi_d[\tilde{\Phi}_d]_m^{-1} = \mathcal{P}^{-1}\Pi_\beta \begin{pmatrix} I_{mm} \\ 0 \end{pmatrix}$$

from (3.45), and then (3.41), $\gamma \to \alpha$ in (3.33), (3.42), and (3.44), respectively. Matrix multiplying on the right by Φ_r^{\dagger} and then substituting for $L_{rb}^{I_r^*}$ from (3.14) leads to (3.46).

Appendix E

E. PROOF OF THEOREM 9

The proof consists of the following two lemmas: Lemma 4 applies directly to the theorem with no change, and Lemma 5 applies with $\tau \to t_1$ and $\widehat{\Omega}_j \to \widehat{\Psi}_j$.

Lemma 4 Under the hypothesis of Theorem 9, applying the biscale perturbation of (4.3) to (4.8) leads to (2.34) for (4.9) and (4.10).

Proof: Substituting (4.8) into (4.3) gives

$$T(\epsilon, \omega_0) = \sum_{j=0}^{J} \mathcal{L}_j [i\omega_0 + \epsilon \partial/\partial t_1]^j$$

$$= \sum_{j=0}^{J} \mathcal{L}_j \left[\sum_{k=0}^{j} \epsilon^k \binom{j}{k} (i\omega_0)^{j-k} \frac{\partial^k}{\partial t_1^k} \right]$$

$$= \sum_{j=0}^{J} \mathcal{L}_j \left[\sum_{k=0}^{J} H_{jk} \epsilon^k \binom{j}{k} (i\omega_0)^{j-k} \frac{\partial^k}{\partial t_1^k} \right]$$

$$= \sum_{k=0}^{J} \epsilon^k \left[\sum_{j=0}^{J} H_{jk} \binom{j}{k} (i\omega_0)^{j-k} \mathcal{L}_j \right] \frac{\partial^k}{\partial t_1^k}$$

$$= \sum_{k=0}^{J} \epsilon^k \left[\sum_{j=k}^{J} \binom{j}{k} (i\omega_0)^{j-k} \mathcal{L}_j \right] \frac{\partial^k}{\partial t_1^k}$$

$$= \sum_{k=0}^{J} \epsilon^k \widehat{T}_k(\omega_0) \frac{\partial^k}{\partial t_1^k}$$

$$= \sum_{k=0}^{J} \epsilon^k T_k$$

when using a binomial expansion (exact because it is finite), the definition (2.38) of H_{jk} twice, (4.10), and (4.9), respectively.

Lemma 5 If Ω_i satisfies (2.61) and

$$T_j = \hat{T}_j \frac{\partial^j}{\partial \tau^j} \tag{E.1}$$

$$\frac{\partial^k}{\partial \tau^k} \hat{T}_j = \hat{T}_j \frac{\partial^k}{\partial \tau^k}$$
 (E.2)

for $0 \le k < \infty$ for each j of $0 \le j \le J$, then

$$\Omega_j = \hat{\Omega}_j \frac{\partial^j}{\partial \tau^j}$$
 (E.3)

$$\frac{\partial^k}{\partial \tau^k} \widehat{\Omega}_j = \widehat{\Omega}_j \frac{\partial^k}{\partial \tau^k} \tag{E.4}$$

for $0 \le k < \infty$ for each j of $0 \le j \le M$, where the $\widehat{\Omega}_j$ component operators are recursively given by

$$\hat{\Omega}_{j} = H_{0j}\hat{T}_{0}^{-1} - \sum_{k=1}^{J} H_{jk}\hat{T}_{0}^{-1}\hat{T}_{k}\hat{\Omega}_{j-k}.$$
(E.5)

Proof: Equation (E.1) for j=0 gives $T_0=\hat{T}_0$ and $T_0^{-1}=\hat{T}_0^{-1}$. Operating on both sides of (E.2) with j=0 by \hat{T}_0^{-1} leads to

$$\frac{\partial^k}{\partial \tau^k} \hat{T}_0^{-1} = \hat{T}_0^{-1} \frac{\partial^k}{\partial \tau^k}.$$
 (E.6)

which shows that (E.4) is true for j=0 when using $\hat{\Omega}_0=\hat{T}_0^{-1}$ from (E.5). For j=0, equation (2.61) gives $\Omega_0=T_0^{-1}$, which combines with $\hat{\Omega}_0=\hat{T}_0^{-1}$ and $T_0^{-1}=\hat{T}_0^{-1}$ to give $\Omega_0=\hat{\Omega}_0$, in agreement with (E.3) for j=0. Equation (E.3) is also true for j=0. To prove (E.4) by induction, take $j\to m$ in (E.5) for m>0 and operate from the left by the linear operator $\partial^k/\partial\tau^k$ to get

$$\frac{\partial^{k}}{\partial \tau^{k}} \hat{\Omega}_{m} = \frac{\partial^{k}}{\partial \tau^{k}} \left(-\left[\sum_{k=1}^{J} H_{mk} \hat{T}_{0}^{-1} \hat{T}_{k} \hat{\Omega}_{m-k} \right] \right)
= -\left[\sum_{k=1}^{J} H_{mk} \hat{T}_{0}^{-1} \frac{\partial^{k}}{\partial \tau^{k}} \hat{T}_{k} \hat{\Omega}_{m-k} \right]
= -\left[\sum_{k=1}^{J} H_{mk} \hat{T}_{0}^{-1} \hat{T}_{k} \frac{\partial^{k}}{\partial \tau^{k}} \hat{\Omega}_{m-k} \right]
= -\left[\sum_{k=1}^{J} H_{mk} \hat{T}_{0}^{-1} \hat{T}_{k} \hat{\Omega}_{m-k} \right] \frac{\partial^{k}}{\partial \tau^{k}}
= \hat{\Omega}_{m} \frac{\partial^{k}}{\partial \tau^{k}}$$

when using (E.6), (E.2) for j=k, (E.4) for all $j\leq m-1$, and $j\to m$ in (E.5) for m>0 again, respectively. Equation (E.4) is proven by induction if the $\hat{\Omega}_j$ component operators are given by (E.5). To prove (E.3) by induction, assume that (E.3) is true for all $j\leq m-1$ (proven for j=0) for some finite m>0. Equation (2.61) and m>0 give

$$\Omega_{m} = -\sum_{k=1}^{J} H_{mk} T_{0}^{-1} T_{k} \Omega_{m-k}
= -\sum_{k=1}^{J} H_{mk} T_{0}^{-1} T_{k} \widehat{\Omega}_{m-k} \frac{\partial^{m-k}}{\partial \tau^{m-k}}
= -\sum_{k=1}^{J} H_{mk} T_{0}^{-1} \widehat{T}_{k} \frac{\partial^{k}}{\partial \tau^{k}} \widehat{\Omega}_{m-k} \frac{\partial^{m-k}}{\partial \tau^{m-k}}
= -\sum_{k=1}^{J} H_{mk} T_{0}^{-1} \widehat{T}_{k} \widehat{\Omega}_{m-k} \frac{\partial^{m}}{\partial \tau^{m}}
= -[\sum_{k=1}^{J} H_{mk} \widehat{T}_{0}^{-1} \widehat{T}_{k} \widehat{\Omega}_{m-k}] \frac{\partial^{m}}{\partial \tau^{m}}
= \widehat{\Omega}_{m} \frac{\partial^{m}}{\partial \tau^{m}}$$

when using (E.3) for all $j \leq m-1$, (E.1), (E.4) for all $j \leq m-1$, $T_0^{-1} = \hat{T}_0^{-1}$, and (E.5) for m>0, respectively. Equation (E.3) is also proven by induction if the $\hat{\Omega}_j$ component operators are given by (E.5).